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Other: ONLINE: WPI, EPODOC, JAPIO,MEDLINE,
BIOSIS, EMBASE, SCISEARCH, CAPLUS

(54) Abstract Title
Crystals of glucokinase and methods of growing them

(57) Crystalline forms of mammalian Glucokinase of sufficient size and quality to obtain structure data by X-ray crystallography are presented. Methods of growing such crystals are also disclosed.

GB 2 385 328 A

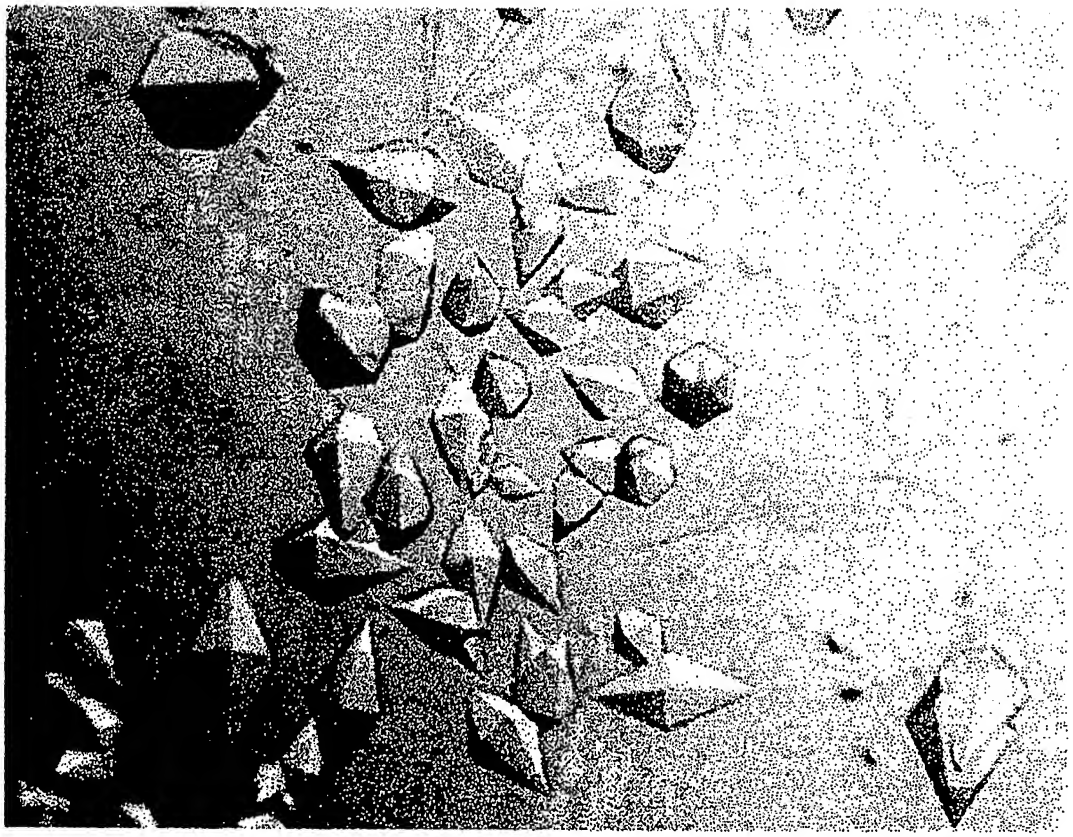

Figure 1

Figure 2. The amino-acid sequence of the GST-GK fusion protein. The GST sequence was taken from GenBank entry U13852. Residue 229 of the fusion protein is the first residue of GK.

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  1 MSPILGYWKI KGLVQPTRLL LEYLEEKYEE HLYERDEGDK WRNKKFELGL EFPNLPYYID
 61 GDVKLTQSMA IIRYIADKHN MLGGCPKERA EISMLEGAVL DIRYGVSRIA YSKDFETLKV
121 DFLSKLPEML KMFEDRLCHK TYLNGDHVTH PDFMLYDALD VVLYMDPMCL DAFPKLVCFK
181 KRIEAIPQID KYLKSSKYIA WPLQGWQATF GGGDHPPKSD LIEGRGIHMP RPRSQLPQPN
241 SQVEQILAEF QLQEEDLKKV MRRMQKEMDR GLRLETHEEA SVKMLPTYVR STPEGSEVGD
301 FLSLDLGGTN FRVMLVKVGE GEEGQWSVKT KHQMYSIPED AMTGTAEMLF DYISECISDF
361 LDKHQMKHKK LPLGFTFSFP VRHEDIDKGI LLNWTKGFKA SGAEGNNVVG LLRDAIKRRG
421 DFEMDVVAMV NDTVATMISC YYEDHQCEVG MIVGTGCNAC YMEEMQNVEL VEGDEGRMCV
481 NTEWGAFGDS GELDEFLLEY DRLVDESSAN PGQQLYEKLI GGKYMGELVR LVLLRLVDEN
541 LLFHGEASEQ LRTRGAFETR FVSQVESDTG DRKQIYNILS TLGLRPSTTD CDIVRRACES
601 VSTRAAHMCS AGLAGVINRM RESRSEDVMR ITVGVDGSVY KLHPSFKERF HASVRRLTPS
661 CEITFIESEE GSGRGAALVS AVACKKACML GQ
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Figure 3

Figure 4

Atom No.	Atom Type		A.A. Type	A.A.#	X	Y	Z	OCC	B
ATOM	1	CB	SER	8	-0.421	63.744	24.899	1.00	50.68
ATOM	2	OG	SER	8	-0.752	63.605	23.524	1.00	50.85
ATOM	3	C	SER	8	1.865	64.216	24.094	1.00	50.72
ATOM	4	O	SER	8	2.308	63.644	23.102	1.00	51.79
ATOM	5	N	SER	8	1.473	63.793	26.507	1.00	50.36
ATOM	6	CA	SER	8	1.057	63.446	25.120	1.00	50.55
ATOM	7	N	GLN	9	2.041	65.515	24.314	1.00	49.84
ATOM	8	CA	GLN	9	2.831	66.312	23.385	1.00	48.95
ATOM	9	CB	GLN	9	2.983	67.745	23.895	1.00	49.08
ATOM	10	CG	GLN	9	3.676	68.686	22.925	1.00	50.25
ATOM	11	CD	GLN	9	3.206	70.127	23.085	1.00	51.06
ATOM	12	OE1	GLN	9	2.037	70.433	22.846	1.00	51.38
ATOM	13	NE2	GLN	9	4.112	71.017	23.499	1.00	51.44
ATOM	14	C	GLN	9	4.190	65.633	23.294	1.00	48.56
ATOM	15	O	GLN	9	4.884	65.741	22.285	1.00	48.75
ATOM	16	N	VAL	10	4.560	64.926	24.361	1.00	47.77
ATOM	17	CA	VAL	10	5.823	64.198	24.392	1.00	46.87
ATOM	18	CB	VAL	10	6.293	63.902	25.842	1.00	46.39
ATOM	19	CG1	VAL	10	7.303	62.782	25.841	1.00	46.41
ATOM	20	CG2	VAL	10	6.952	65.135	26.436	1.00	46.79
ATOM	21	C	VAL	10	5.616	62.885	23.653	1.00	46.17
ATOM	22	O	VAL	10	6.521	62.384	22.991	1.00	46.18
ATOM	23	N	GLU	11	4.423	62.317	23.768	1.00	45.28
ATOM	24	CA	GLU	11	4.159	61.071	23.069	1.00	45.19
ATOM	25	CB	GLU	11	2.905	60.393	23.616	1.00	45.21
ATOM	26	CG	GLU	11	3.105	59.709	24.967	1.00	46.05
ATOM	27	CD	GLU	11	4.224	58.664	24.957	1.00	46.30
ATOM	28	OE1	GLU	11	4.350	57.918	23.948	1.00	46.28
ATOM	29	OE2	GLU	11	4.963	58.583	25.972	1.00	45.66
ATOM	30	C	GLU	11	4.002	61.345	21.580	1.00	44.48
ATOM	31	O	GLU	11	4.068	60.430	20.755	1.00	44.48
ATOM	32	N	GLN	12	3.807	62.614	21.239	1.00	43.86
ATOM	33	CA	GLN	12	3.646	62.996	19.845	1.00	42.86
ATOM	34	CB	GLN	12	2.972	64.368	19.715	1.00	44.49
ATOM	35	CG	GLN	12	2.833	64.840	18.259	1.00	46.49
ATOM	36	CD	GLN	12	1.986	66.099	18.113	1.00	47.74
ATOM	37	OE1	GLN	12	2.055	66.799	17.088	1.00	48.30
ATOM	38	NE2	GLN	12	1.174	66.388	19.131	1.00	47.51
ATOM	39	C	GLN	12	5.014	63.023	19.192	1.00	41.14
ATOM	40	O	GLN	12	5.139	62.739	18.002	1.00	41.76
ATOM	41	N	ILE	13	6.038	63.360	19.971	1.00	38.51
ATOM	42	CA	ILE	13	7.398	63.388	19.450	1.00	36.48
ATOM	43	CB	ILE	13	8.274	64.351	20.261	1.00	35.85
ATOM	44	CG2	ILE	13	9.731	64.228	19.827	1.00	35.71
ATOM	45	CG1	ILE	13	7.740	65.777	20.079	1.00	35.77
ATOM	46	CD1	ILE	13	8.584	66.867	20.710	1.00	35.91
ATOM	47	C	ILE	13	8.018	61.981	19.452	1.00	36.01
ATOM	48	O	ILE	13	8.572	61.528	18.442	1.00	35.99
ATOM	49	N	LEU	14	7.903	61.288	20.580	1.00	34.88
ATOM	50	CA	LEU	14	8.430	59.934	20.711	1.00	33.91
ATOM	51	CB	LEU	14	8.230	59.432	22.141	1.00	33.29
ATOM	52	CG	LEU	14	8.853	60.321	23.215	1.00	33.43
ATOM	53	CD1	LEU	14	8.510	59.781	24.594	1.00	33.04
ATOM	54	CD2	LEU	14	10.354	60.398	23.001	1.00	33.04

Figure 4

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ATOM     55  C   LEU  14      7.766  58.957  19.730  1.00 33.55
ATOM     56  O   LEU  14      8.208  57.812  19.578  1.00 33.21
ATOM     57  N   ALA  15      6.710  59.403  19.065  1.00 32.69
ATOM     58  CA  ALA  15      6.021  58.551  18.104  1.00 32.59
ATOM     59  CB  ALA  15      4.628  59.104  17.821  1.00 31.95
ATOM     60  C   ALA  15      6.838  58.449  16.808  1.00 32.79
ATOM     61  O   ALA  15      6.664  57.519  16.018  1.00 33.05
ATOM     62  N   GLU  16      7.746  59.395  16.599  1.00 32.33
ATOM     63  CA  GLU  16      8.575  59.369  15.403  1.00 32.74
ATOM     64  CB  GLU  16      9.566  60.531  15.401  1.00 34.23
ATOM     65  CG  GLU  16      8.950  61.910  15.298  1.00 38.39
ATOM     66  CD  GLU  16     10.017  62.998  15.162  1.00 41.11
ATOM     67  OE1 GLU  16     10.445  63.269  14.012  1.00 40.68
ATOM     68  OE2 GLU  16     10.438  63.562  16.212  1.00 42.77
ATOM     69  C   GLU  16      9.369  58.073  15.279  1.00 31.93
ATOM     70  O   GLU  16      9.570  57.568  14.179  1.00 33.41
ATOM     71  N   PHE  17      9.841  57.539  16.401  1.00 30.37
ATOM     72  CA  PHE  17     10.640  56.321  16.369  1.00 27.71
ATOM     73  CB  PHE  17     11.346  56.129  17.711  1.00 26.32
ATOM     74  CG  PHE  17     12.309  57.230  18.045  1.00 24.22
ATOM     75  CD1 PHE  17     11.846  58.500  18.389  1.00 23.88
ATOM     76  CD2 PHE  17     13.680  57.010  17.981  1.00 22.24
ATOM     77  CE1 PHE  17     12.741  59.531  18.660  1.00 22.63
ATOM     78  CE2 PHE  17     14.574  58.027  18.250  1.00 21.23
ATOM     79  CZ  PHE  17     14.105  59.291  18.589  1.00 22.01
ATOM     80  C   PHE  17      9.836  55. 004  077  16.012  1.00 27.77
ATOM     81  O   PHE  17     10.400  54. 15.802  1.00 27.38
ATOM     82  N   GLN  18      8.517  55.213  15.957  1.00 28.12
ATOM     83  CA  GLN  18      7.684  54.080  15.593  1.00 29.17
ATOM     84  CB  GLN  18      6.216  54.484  15.599  1.00 30.98
ATOM     85  CG  GLN  18      5.446  54.017  16.806  1.00 32.94
ATOM     86  CD  GLN  18      4.152  54.785  16.974  1.00 34.65
ATOM     87  OE1 GLN  18      3.389  54.976  16.014  1.00 37.17
ATOM     88  NE2 GLN  18      3.892  55.228  18.190  1.00 33.67
ATOM     89  C   GLN  18      8.068  53.602  14.193  1.00 28.97
ATOM     90  O   GLN  18      8.471  54.399  13.346  1.00 28.83
ATOM     91  N   LEU  19      7.931  52.298  13.971  1.00 29.02
ATOM     92  CA  LEU  19      8.235  51.659  12.704  1.00 29.94
ATOM     93  CB  LEU  19      9.641  51.069  12.749  1.00 29.78
ATOM     94  CG  LEU  19     10.782  51.813  12.037  1.00 30.77
ATOM     95  CD1 LEU  19     10.886  53.251  12.477  1.00 30.67
ATOM     96  CD2 LEU  19     12.083  51.087  12.339  1.00 32.05
ATOM     97  C   LEU  19      7.199  50.549  12.511  1.00 31.41
ATOM     98  O   LEU  19      7.288  49.484  13.137  1.00 31.35
ATOM     99  N   GLN  20      6.205  50.801  11.663  1.00 32.64
ATOM    100  CA  GLN  20      5.153  49.817  11.422  1.00 34.95
ATOM    101  CB  GLN  20      4.024  50.413  10.570  1.00 35.78
ATOM    102  CG  GLN  20      3.301  51.622  11.175  1.00 37.65
ATOM    103  CD  GLN  20      3.048  51.486  12.669  1.00 39.03
ATOM    104  OE1 GLN  20      2.603  50.441  13.152  1.00 40.92
ATOM    105  NE2 GLN  20      3.324  52.552  13.410  1.00 40.04
ATOM    106  C   GLN  20      5.692  48.568  10.730  1.00 35.83
ATOM    107  O   GLN  20      6.827  48.547  10.247  1.00 36.56
ATOM    108  N   GLU  21      4.864  47.531  10.681  1.00 36.52
ATOM    109  CA  GLU  21      5.240  46.279  10.062  1.00 37.80
ATOM    110  CB  GLU  21      4.024  45.357   9.998  1.00 39.22
ATOM    111  CG  GLU  21      4.298  43.898   9.625  1.00 42.88
ATOM    112  CD  GLU  21      4.568  43.009  10.844  1.00 44.63
ATOM    113  OE1 GLU  21      4.540  41.758  10.699  1.00 45.40
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Figure 4

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ATOM    114  OE2 GLU    21       4.810  43.564  11.943  1.00 45.89
ATOM    115  C   GLU    21       5.770  46.549   8.654  1.00 38.20
ATOM    116  O   GLU    21       6.892  46.183   8.324  1.00 38.71
ATOM    117  N   GLU    22       4.972  47.208   7.826  1.00 38.54
ATOM    118  CA  GLU    22       5.386  47.478   6.457  1.00 39.08
ATOM    119  CB  GLU    22       4.308  48.267   5.703  1.00 40.61
ATOM    120  CG  GLU    22       3.123  47.406   5.313  1.00 43.51
ATOM    121  CD  GLU    22       3.556  46.039   4.773  1.00 45.80
ATOM    122  OE1 GLU    22       4.243  45.999   3.719  1.00 46.20
ATOM    123  OE2 GLU    22       3.215  45.007   5.414  1.00 46.87
ATOM    124  C   GLU    22       6.711  48.197   6.359  1.00 38.74
ATOM    125  O   GLU    22       7.482  47.954   5.423  1.00 39.26
ATOM    126  N   ASP    23       6.988  49.084   7.308  1.00 37.74
ATOM    127  CA  ASP    23       8.258  49.795   7.276  1.00 37.23
ATOM    128  CB  ASP    23       8.356  50.779   8.437  1.00 38.62
ATOM    129  CG  ASP    23       7.240  51.789   8.427  1.00 40.46
ATOM    130  OD1 ASP    23       7.104  52.508   7.408  1.00 41.26
ATOM    131  OD2 ASP    23       6.495  51.861   9.438  1.00 41.77
ATOM    132  C   ASP    23       9.371  48.760   7.382  1.00 35.54
ATOM    133  O   ASP    23      10.267  48.698   6.536  1.00 35.43
ATOM    134  N   LEU    24       9.294  47.937   8.420  1.00 33.31
ATOM    135  CA  LEU    24      10.288  46.910   8.631  1.00 32.04
ATOM    136  CB  LEU    24       9.898  46.062   9.842  1.00 31.35
ATOM    137  CG  LEU    24       9.920  46.801  11.196  1.00 31.20
ATOM    138  CD1 LEU    24       9.710  45.815  12.343  1.00 29.48
ATOM    139  CD2 LEU    24      11.253  47.526  11.367  1.00 31.51
ATOM    140  C   LEU    24      10.509  46.041   7.385  1.00 31.61
ATOM    141  O   LEU    24      11.645  45.723   7.049  1.00 31.67
ATOM    142  N   LYS    25       9.434  45.673   6.693  1.00 31.58
ATOM    143  CA  LYS    25       9.551  44.863   5.486  1.00 31.41
ATOM    144  CB  LYS    25       8.186  44.347   5.061  1.00 31.91
ATOM    145  CG  LYS    25       7.574  43.372   6.033  1.00 34.39
ATOM    146  CD  LYS    25       6.224  42.901   5.531  1.00 36.61
ATOM    147  CE  LYS    25       5.414  42.232   6.640  1.00 38.71
ATOM    148  NZ  LYS    25       3.978  42.086   6.235  1.00 39.39
ATOM    149  C   LYS    25      10.166  45.679   4.352  1.00 31.50
ATOM    150  O   LYS    25      10.969  45.170   3.568  1.00 30.92
ATOM    151  N   LYS    26       9.784  46.947   4.261  1.00 31.82
ATOM    152  CA  LYS    26      10.332  47.819   3.229  1.00 32.63
ATOM    153  CB  LYS    26       9.695  49.203   3.315  1.00 33.38
ATOM    154  CG  LYS    26      10.053  50.129   2.177  1.00 35.11
ATOM    155  CD  LYS    26       9.424  51.502   2.400  1.00 37.48
ATOM    156  CE  LYS    26       9.364  52.312   1.104  1.00 39.72
ATOM    157  NZ  LYS    26       8.706  53.645   1.307  1.00 42.62
ATOM    158  C   LYS    26      11.845  47.919   3.441  1.00 32.91
ATOM    159  O   LYS    26      12.614  48.012   2.479  1.00 32.90
ATOM    160  N   VAL    27      12.265  47.901   4.705  1.00 33.16
ATOM    161  CA  VAL    27      13.687  47.956   5.046  1.00 33.43
ATOM    162  CB  VAL    27      13.903  48.281   6.555  1.00 32.58
ATOM    163  CG1 VAL    27      15.335  47.960   6.963  1.00 32.13
ATOM    164  CG2 VAL    27      13.622  49.755   6.818  1.00 31.04
ATOM    165  C   VAL    27      14.305  46.586   4.727  1.00 33.90
ATOM    166  O   VAL    27      15.323  46.482   4.036  1.00 33.83
ATOM    167  N   MSE    28      13.668  45.536   5.223  1.00 34.26
ATOM    168  CA  MSE    28      14.140  44.193   4.983  1.00 34.84
ATOM    169  CB  MSE    28      13.072  43.198   5.393  1.00 35.83
ATOM    170  CG  MSE    28      13.456  41.784   5.144  1.00 38.88
ATOM    171  SE  MSE    28      12.108  40.670   5.608  1.00 45.40
ATOM    172  CE  MSE    28      11.054  40.713   4.095  1.00 42.96
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Figure 4

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ATOM    173  C   MSE  28      14.465  44.016   3.505  1.00 35.32
ATOM    174  O   MSE  28      15.571  43.621   3.144  1.00 35.22
ATOM    175  N   ARG  29      13.495  44.331   2.655  1.00 36.22
ATOM    176  CA  ARG  29      13.665  44.191   1.218  1.00 36.59
ATOM    177  CB  ARG  29      12.352  44.520   0.509  1.00 37.37
ATOM    178  CG  ARG  29      11.223  43.542   0.827  1.00 38.96
ATOM    179  CD  ARG  29       9.913  43.960   0.152  1.00 40.89
ATOM    180  NE  ARG  29       8.760  43.281   0.744  1.00 42.88
ATOM    181  CZ  ARG  29       7.621  43.889   1.081  1.00 43.80
ATOM    182  NH1 ARG  29       7.475  45.201   0.881  1.00 43.07
ATOM    183  NH2 ARG  29       6.631  43.188   1.636  1.00 44.12
ATOM    184  C   ARG  29      14.814  45.008   0.625  1.00 36.30
ATOM    185  O   ARG  29      15.615  44.469  -0.133  1.00 35.58
ATOM    186  N   ARG  30      14.906  46.296   0.948  1.00 36.85
ATOM    187  CA  ARG  30      16.008  47.091   0.410  1.00 38.41
ATOM    188  CB  ARG  30      15.944  48.543   0.894  1.00 39.31
ATOM    189  CG  ARG  30      14.676  49.285   0.513  1.00 41.96
ATOM    190  CD  ARG  30      14.742  50.763   0.933  1.00 44.07
ATOM    191  NE  ARG  30      13.415  51.384   0.995  1.00 45.48
ATOM    192  CZ  ARG  30      13.179  52.628   1.416  1.00 45.93
ATOM    193  NH1 ARG  30      14.175  53.403   1.810  1.00 45.92
ATOM    194  NH2 ARG  30      11.937  53.091   1.467  1.00 45.68
ATOM    195  C   ARG  30      17.338  46.461   0.843  1.00 39.05
ATOM    196  O   ARG  30      18.286  46.404   0.061  1.00 38.99
ATOM    197  N   MSE  31      17.408  45.999   2.092  1.00 39.11
ATOM    198  CA  MSE  31      18.615  45.348   2.596  1.00 38.96
ATOM    199  CB  MSE  31      18.374  44.784   4.002  1.00 40.43
ATOM    200  CG  MSE  31      19.512  43.922   4.599  1.00 42.62
ATOM    201  SE  MSE  31      21.083  44.819   5.027  1.00 48.46
ATOM    202  CE  MSE  31      20.438  45.988   6.389  1.00 45.46
ATOM    203  C   MSE  31      18.901  44.209   1.633  1.00 38.25
ATOM    204  O   MSE  31      19.973  44.132   1.038  1.00 38.18
ATOM    205  N   GLN  32      17.915  43.334   1.478  1.00 37.93
ATOM    206  CA  GLN  32      18.037  42.199   0.589  1.00 37.33
ATOM    207  CB  GLN  32      16.708  41.475   0.480  1.00 36.41
ATOM    208  CG  GLN  32      16.219  40.905   1.780  1.00 37.04
ATOM    209  CD  GLN  32      15.304  39.723   1.561  1.00 37.28
ATOM    210  OE1 GLN  32      15.740  38.682   1.072  1.00 38.23
ATOM    211  NE2 GLN  32      14.027  39.874   1.912  1.00 37.39
ATOM    212  C   GLN  32      18.475  42.641  -0.791  1.00 37.81
ATOM    213  O   GLN  32      19.215  41.929  -1.466  1.00 37.79
ATOM    214  N   LYS  33      18.019  43.819  -1.205  1.00 38.80
ATOM    215  CA  LYS  33      18.362  44.345  -2.516  1.00 39.85
ATOM    216  CB  LYS  33      17.525  45.588  -2.830  1.00 40.63
ATOM    217  CG  LYS  33      17.591  45.992  -4.298  1.00 42.21
ATOM    218  CD  LYS  33      16.924  47.336  -4.561  1.00 43.78
ATOM    219  CE  LYS  33      17.160  47.803  -6.006  1.00 44.42
ATOM    220  NZ  LYS  33      16.639  49.187  -6.256  1.00 44.23
ATOM    221  C   LYS  33      19.843  44.695  -2.574  1.00 40.37
ATOM    222  O   LYS  33      20.519  44.411  -3.564  1.00 40.53
ATOM    223  N   GLU  34      20.331  45.312  -1.500  1.00 40.59
ATOM    224  CA  GLU  34      21.730  45.712  -1.378  1.00 40.95
ATOM    225  CB  GLU  34      21.912  46.641  -0.179  1.00 41.24
ATOM    226  CG  GLU  34      21.229  47.956  -0.359  1.00 41.42
ATOM    227  CD  GLU  34      21.476  48.506  -1.741  1.00 42.21
ATOM    228  OE1 GLU  34      22.650  48.810  -2.063  1.00 42.30
ATOM    229  OE2 GLU  34      20.493  48.613  -2.507  1.00 43.29
ATOM    230  C   GLU  34      22.667  44.528  -1.221  1.00 40.87
ATOM    231  O   GLU  34      23.770  44.527  -1.767  1.00 41.06
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ATOM    232  N   MSE   35      22.233  43.534  -0.456  1.00 41.15
ATOM    233  CA  MSE   35      23.038  42.350  -0.232  1.00 41.36
ATOM    234  CB  MSE   35      22.289  41.354   0.648  1.00 41.62
ATOM    235  CG  MSE   35      22.320  41.711   2.117  1.00 43.28
ATOM    236  SE  MSE   35      21.428  40.506   3.120  1.00 46.51
ATOM    237  CE  MSE   35      22.217  38.947   2.587  1.00 45.63
ATOM    238  C   MSE   35      23.376  41.701  -1.554  1.00 41.91
ATOM    239  O   MSE   35      24.532  41.367  -1.824  1.00 42.73
ATOM    240  N   ASP   36      22.367  41.533  -2.395  1.00 42.15
ATOM    241  CA  ASP   36      22.593  40.898  -3.675  1.00 41.96
ATOM    242  CB  ASP   36      21.264  40.633  -4.369  1.00 43.56
ATOM    243  CG  ASP   36      21.446  39.947  -5.699  1.00 45.91
ATOM    244  OD1 ASP   36      21.821  40.652  -6.675  1.00 46.71
ATOM    245  OD2 ASP   36      21.232  38.707  -5.754  1.00 46.76
ATOM    246  C   ASP   36      23.502  41.717  -4.578  1.00 41.03
ATOM    247  O   ASP   36      24.406  41.178  -5.217  1.00 40.61
ATOM    248  N   ARG   37      23.257  43.021  -4.620  1.00 40.36
ATOM    249  CA  ARG   37      24.034  43.937  -5.446  1.00 39.76
ATOM    250  CB  ARG   37      23.498  45.355  -5.283  1.00 39.56
ATOM    251  CG  ARG   37      22.252  45.621  -6.112  1.00 40.04
ATOM    252  CD  ARG   37      21.465  46.815  -5.590  1.00 41.19
ATOM    253  NE  ARG   37      22.278  48.002  -5.307  1.00 41.70
ATOM    254  CZ  ARG   37      22.938  48.711  -6.221  1.00 42.38
ATOM    255  NH1 ARG   37      22.899  48.362  -7.505  1.00 42.59
ATOM    256  NH2 ARG   37      23.615  49.792  -5.851  1.00 41.94
ATOM    257  C   ARG   37      25.524  43.908  -5.152  1.00 39.94
ATOM    258  O   ARG   37      26.335  43.732  -6.059  1.00 40.39
ATOM    259  N   GLY   38      25.893  44.076  -3.890  1.00 39.94
ATOM    260  CA  GLY   38      27.305  44.063  -3.557  1.00 39.60
ATOM    261  C   GLY   38      27.933  42.689  -3.699  1.00 39.23
ATOM    262  O   GLY   38      29.163  42.546  -3.695  1.00 39.59
ATOM    263  N   LEU   39      27.087  41.677  -3.834  1.00 38.16
ATOM    264  CA  LEU   39      27.545  40.307  -3.960  1.00 37.65
ATOM    265  CB  LEU   39      26.428  39.376  -3.495  1.00 35.76
ATOM    266  CG  LEU   39      26.821  38.029  -2.900  1.00 34.52
ATOM    267  CD1 LEU   39      27.899  38.248  -1.857  1.00 33.52
ATOM    268  CD2 LEU   39      25.606  37.348  -2.284  1.00 32.44
ATOM    269  C   LEU   39      27.931  39.989  -5.407  1.00 39.20
ATOM    270  O   LEU   39      28.594  38.980  -5.681  1.00 39.88
ATOM    271  N   ARG   40      27.537  40.866  -6.329  1.00 40.51
ATOM    272  CA  ARG   40      27.809  40.656  -7.751  1.00 41.77
ATOM    273  CB  ARG   40      26.494  40.686  -8.526  1.00 42.80
ATOM    274  CG  ARG   40      25.735  39.392  -8.377  1.00 44.75
ATOM    275  CD  ARG   40      24.257  39.551  -8.636  1.00 46.47
ATOM    276  NE  ARG   40      23.639  38.239  -8.797  1.00 48.71
ATOM    277  CZ  ARG   40      22.331  38.034  -8.890  1.00 50.01
ATOM    278  NH1 ARG   40      21.497  39.064  -8.831  1.00 51.43
ATOM    279  NH2 ARG   40      21.861  36.804  -9.060  1.00 50.46
ATOM    280  C   ARG   40      28.802  41.623  -8.374  1.00 42.16
ATOM    281  O   ARG   40      28.783  42.819  -8.097  1.00 42.42
ATOM    282  N   LEU   41      29.650  41.087  -9.247  1.00 42.03
ATOM    283  CA  LEU   41      30.689  41.864  -9.902  1.00 42.00
ATOM    284  CB  LEU   41      31.307  41.044 -11.041  1.00 42.00
ATOM    285  CG  LEU   41      32.577  41.650 -11.660  1.00 41.78
ATOM    286  CD1 LEU   41      33.638  41.836 -10.583  1.00 40.20
ATOM    287  CD2 LEU   41      33.087  40.747 -12.773  1.00 41.95
ATOM    288  C   LEU   41      30.278  43.237 -10.428  1.00 42.57
ATOM    289  O   LEU   41      30.920  44.243 -10.110  1.00 42.64
ATOM    290  N   GLU   42      29.219  43.292 -11.227  1.00 43.03
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Figure 4

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ATOM    291  CA  GLU    42      28.788  44.562 -11.803  1.00 44.63
ATOM    292  CB  GLU    42      27.494  44.369 -12.607  1.00 43.97
ATOM    293  CG  GLU    42      26.436  43.533 -11.922  1.00 44.02
ATOM    294  CD  GLU    42      26.546  42.057 -12.248  1.00 43.71
ATOM    295  OE1 GLU    42      27.673  41.527 -12.245  1.00 45.13
ATOM    296  OE2 GLU    42      25.504  41.416 -12.496  1.00 43.50
ATOM    297  C   GLU    42      28.616  45.714 -10.805  1.00 46.21
ATOM    298  O   GLU    42      28.963  46.860 -11.103  1.00 46.22
ATOM    299  N   THR    43      28.105  45.413  -9.616  1.00 47.90
ATOM    300  CA  THR    43      27.873  46.443  -8.608  1.00 49.10
ATOM    301  CB  THR    43      26.370  46.533  -8.285  1.00 48.63
ATOM    302  OG1 THR    43      25.772  45.242  -8.465  1.00 47.66
ATOM    303  CG2 THR    43      25.679  47.531  -9.192  1.00 48.90
ATOM    304  C   THR    43      28.629  46.226  -7.302  1.00 50.94
ATOM    305  O   THR    43      28.481  47.008  -6.362  1.00 51.52
ATOM    306  N   HIS    44      29.456  45.185  -7.249  1.00 52.58
ATOM    307  CA  HIS    44      30.204  44.854  -6.037  1.00 53.89
ATOM    308  CB  HIS    44      31.210  43.727  -6.311  1.00 54.68
ATOM    309  CG  HIS    44      32.552  44.208  -6.775  1.00 55.77
ATOM    310  CD2 HIS    44      33.748  44.257  -6.139  1.00 55.82
ATOM    311  ND1 HIS    44      32.758  44.772  -8.017  1.00 56.36
ATOM    312  CE1 HIS    44      34.020  45.146  -8.125  1.00 56.30
ATOM    313  NE2 HIS    44      34.643  44.845  -6.999  1.00 56.06
ATOM    314  C   HIS    44      30.950  46.013  -5.398  1.00 54.87
ATOM    315  O   HIS    44      30.823  46.254  -4.199  1.00 55.06
ATOM    316  N   GLU    45      31.724  46.732  -6.203  1.00 56.25
ATOM    317  CA  GLU    45      32.540  47.826  -5.703  1.00 57.17
ATOM    318  CB  GLU    45      33.618  48.180  -6.721  1.00 59.35
ATOM    319  CG  GLU    45      33.146  49.127  -7.800  1.00 61.61
ATOM    320  CD  GLU    45      34.107  50.279  -7.985  1.00 63.07
ATOM    321  OE1 GLU    45      35.228  50.038  -8.487  1.00 63.72
ATOM    322  OE2 GLU    45      33.747  51.420  -7.613  1.00 64.00
ATOM    323  C   GLU    45      31.762  49.074  -5.356  1.00 56.66
ATOM    324  O   GLU    45      32.295  49.985  -4.732  1.00 56.54
ATOM    325  N   GLU    46      30.508  49.135  -5.772  1.00 56.24
ATOM    326  CA  GLU    46      29.708  50.306  -5.456  1.00 56.37
ATOM    327  CB  GLU    46      29.542  51.157  -6.704  1.00 57.92
ATOM    328  CG  GLU    46      30.881  51.645  -7.212  1.00 60.77
ATOM    329  CD  GLU    46      30.782  52.400  -8.515  1.00 62.28
ATOM    330  OE1 GLU    46      30.566  51.762  -9.571  1.00 62.25
ATOM    331  OE2 GLU    46      30.914  53.641  -8.474  1.00 63.95
ATOM    332  C   GLU    46      28.366  49.891  -4.873  1.00 55.40
ATOM    333  O   GLU    46      27.309  50.123  -5.457  1.00 55.75
ATOM    334  N   ALA    47      28.440  49.264  -3.704  1.00 53.89
ATOM    335  CA  ALA    47      27.273  48.783  -2.987  1.00 51.80
ATOM    336  CB  ALA    47      27.140  47.280  -3.159  1.00 52.36
ATOM    337  C   ALA    47      27.470  49.111  -1.524  1.00 49.98
ATOM    338  O   ALA    47      28.448  48.664  -0.923  1.00 50.36
ATOM    339  N   SER    48      26.553  49.894  -0.960  1.00 47.18
ATOM    340  CA  SER    48      26.630  50.267   0.444  1.00 44.70
ATOM    341  CB  SER    48      25.299  50.860   0.897  1.00 46.13
ATOM    342  OG  SER    48      24.243  49.927   0.720  1.00 47.87
ATOM    343  C   SER    48      26.965  49.041   1.287  1.00 42.45
ATOM    344  O   SER    48      27.841  49.082   2.147  1.00 42.01
ATOM    345  N   VAL    49      26.261  47.946   1.037  1.00 40.48
ATOM    346  CA  VAL    49      26.516  46.713   1.762  1.00 38.96
ATOM    347  CB  VAL    49      25.231  45.849   1.875  1.00 38.62
ATOM    348  CG1 VAL    49      25.496  44.625   2.740  1.00 38.40
ATOM    349  CG2 VAL    49      24.102  46.672   2.472  1.00 37.16
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Figure 4

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ATOM    350  C   VAL  49      27.572  45.997   0.929  1.00 37.97
ATOM    351  O   VAL  49      27.266  45.474  -0.137  1.00 38.42
ATOM    352  N   LYS  50      28.810  45.982   1.422  1.00 36.51
ATOM    353  CA  LYS  50      29.937  45.385   0.703  1.00 34.95
ATOM    354  CB  LYS  50      31.250  45.843   1.334  1.00 35.51
ATOM    355  CG  LYS  50      31.574  47.322   1.091  1.00 36.68
ATOM    356  CD  LYS  50      30.676  48.249   1.913  1.00 39.05
ATOM    357  CE  LYS  50      30.865  48.018   3.419  1.00 39.54
ATOM    358  NZ  LYS  50      32.316  48.157   3.792  1.00 40.04
ATOM    359  C   LYS  50      30.012  43.879   0.482  1.00 33.72
ATOM    360  O   LYS  50      30.845  43.421  -0.293  1.00 33.30
ATOM    361  N   MSE  51      29.171  43.100   1.147  1.00 33.02
ATOM    362  CA  MSE  51      29.209  41.647   0.967  1.00 32.08
ATOM    363  CB  MSE  51      28.291  41.257  -0.190  1.00 34.01
ATOM    364  CG  MSE  51      26.867  41.744  -0.025  1.00 36.03
ATOM    365  SE  MSE  51      26.148  41.146   1.529  1.00 40.73
ATOM    366  CE  MSE  51      25.558  39.411   1.085  1.00 37.98
ATOM    367  C   MSE  51      30.637  41.180   0.666  1.00 30.17
ATOM    368  O   MSE  51      30.928  40.723  -0.437  1.00 30.22
ATOM    369  N   LEU  52      31.518  41.295   1.650  1.00 28.96
ATOM    370  CA  LEU  52      32.920  40.928   1.487  1.00 27.43
ATOM    371  CB  LEU  52      33.769  41.839   2.357  1.00 28.05
ATOM    372  CG  LEU  52      33.649  43.319   1.991  1.00 28.52
ATOM    373  CD1 LEU  52      34.222  44.171   3.116  1.00 28.77
ATOM    374  CD2 LEU  52      34.369  43.583   0.658  1.00 28.75
ATOM    375  C   LEU  52      33.273  39.482   1.803  1.00 26.61
ATOM    376  O   LEU  52      32.997  38.995   2.893  1.00 25.26
ATOM    377  N   PRO  53      33.911  38.774   0.844  1.00 27.04
ATOM    378  CD  PRO  53      34.270  39.142  -0.540  1.00 25.69
ATOM    379  CA  PRO  53      34.264  37.375   1.133  1.00 27.99
ATOM    380  CB  PRO  53      34.807  36.864  -0.204  1.00 26.92
ATOM    381  CG  PRO  53      34.184  37.825  -1.241  1.00 25.77
ATOM    382  C   PRO  53      35.314  37.361   2.239  1.00 28.40
ATOM    383  O   PRO  53      36.152  38.271   2.317  1.00 28.36
ATOM    384  N   THR  54      35.255  36.329   3.080  1.00 29.46
ATOM    385  CA  THR  54      36.149  36.142   4.226  1.00 30.53
ATOM    386  CB  THR  54      35.317  35.951   5.502  1.00 29.48
ATOM    387  OG1 THR  54      34.589  34.711   5.418  1.00 27.97
ATOM    388  CG2 THR  54      34.324  37.084   5.659  1.00 29.42
ATOM    389  C   THR  54      37.018  34.884   4.071  1.00 31.60
ATOM    390  O   THR  54      37.657  34.423   5.025  1.00 32.25
ATOM    391  N   TYR  55      37.017  34.311   2.877  1.00 32.63
ATOM    392  CA  TYR  55      37.763  33.089   2.615  1.00 34.41
ATOM    393  CB  TYR  55      39.249  33.421   2.405  1.00 33.07
ATOM    394  CG  TYR  55      39.458  34.175   1.101  1.00 32.58
ATOM    395  CD1 TYR  55      39.518  35.571   1.067  1.00 32.44
ATOM    396  CE1 TYR  55      39.572  36.263  -0.157  1.00 32.48
ATOM    397  CD2 TYR  55      39.467  33.492  -0.117  1.00 31.97
ATOM    398  CE2 TYR  55      39.516  34.172  -1.335  1.00 31.83
ATOM    399  CZ  TYR  55      39.566  35.548  -1.351  1.00 32.18
ATOM    400  OH  TYR  55      39.575  36.200  -2.568  1.00 32.67
ATOM    401  C   TYR  55      37.559  31.956   3.637  1.00 36.06
ATOM    402  O   TYR  55      38.314  30.991   3.665  1.00 37.61
ATOM    403  N   VAL  56      36.518  32.059   4.459  1.00 38.03
ATOM    404  CA  VAL  56      36.199  31.006   5.429  1.00 39.87
ATOM    405  CB  VAL  56      35.483  31.586   6.663  1.00 38.75
ATOM    406  CG1 VAL  56      35.202  30.492   7.669  1.00 38.10
ATOM    407  CG2 VAL  56      36.336  32.660   7.285  1.00 38.76
ATOM    408  C   VAL  56      35.249  30.032   4.706  1.00 42.20
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Figure 4

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ATOM    409  O   VAL  56      34.098  30.376   4.418  1.00 42.02
ATOM    410  N   ARG  57      35.718  28.821   4.414  1.00 44.49
ATOM    411  CA  ARG  57      34.896  27.860   3.676  1.00 47.07
ATOM    412  CB  ARG  57      35.688  27.288   2.499  1.00 48.02
ATOM    413  CG  ARG  57      36.209  28.310   1.508  1.00 49.08
ATOM    414  CD  ARG  57      36.558  27.626   0.185  1.00 49.69
ATOM    415  NE  ARG  57      37.239  28.528  -0.737  1.00 49.50
ATOM    416  CZ  ARG  57      38.367  29.167  -0.447  1.00 48.83
ATOM    417  NH1 ARG  57      38.938  28.997   0.745  1.00 48.13
ATOM    418  NH2 ARG  57      38.915  29.978  -1.345  1.00 47.51
ATOM    419  C   ARG  57      34.311  26.695   4.449  1.00 48.57
ATOM    420  O   ARG  57      34.810  26.310   5.500  1.00 48.65
ATOM    421  N   SER  58      33.256  26.117   3.891  1.00 51.15
ATOM    422  CA  SER  58      32.589  24.973   4.501  1.00 54.78
ATOM    423  CB  SER  58      31.204  24.793   3.882  1.00 54.26
ATOM    424  OG  SER  58      31.258  24.980   2.475  1.00 54.39
ATOM    425  C   SER  58      33.419  23.708   4.295  1.00 57.39
ATOM    426  O   SER  58      33.097  22.645   4.823  1.00 57.47
ATOM    427  N   THR  59      34.484  23.840   3.510  1.00 60.71
ATOM    428  CA  THR  59      35.392  22.740   3.216  1.00 64.02
ATOM    429  CB  THR  59      35.886  22.823   1.758  1.00 63.73
ATOM    430  OG1 THR  59      36.637  24.029   1.570  1.00 63.22
ATOM    431  CG2 THR  59      34.704  22.843   0.801  1.00 63.87
ATOM    432  C   THR  59      36.571  22.880   4.176  1.00 67.10
ATOM    433  O   THR  59      37.554  23.562   3.884  1.00 67.44
ATOM    434  N   PRO  60      36.480  22.238   5.349  1.00 69.75
ATOM    435  CD  PRO  60      35.366  21.412   5.854  1.00 70.63
ATOM    436  CA  PRO  60      37.556  22.320   6.337  1.00 71.72
ATOM    437  CB  PRO  60      36.841  21.982   7.636  1.00 71.72
ATOM    438  CG  PRO  60      35.909  20.881   7.182  1.00 71.50
ATOM    439  C   PRO  60      38.709  21.370   6.056  1.00 73.48
ATOM    440  O   PRO  60      39.522  21.609   5.158  1.00 73.53
ATOM    441  N   GLU  61      38.754  20.287   6.830  1.00 75.48
ATOM    442  CA  GLU  61      39.808  19.283   6.731  1.00 76.98
ATOM    443  CB  GLU  61      39.969  18.788   5.289  1.00 78.43
ATOM    444  CG  GLU  61      40.806  17.516   5.161  1.00 80.68
ATOM    445  CD  GLU  61      42.177  17.744   4.530  1.00 81.88
ATOM    446  OE1 GLU  61      42.993  18.498   5.100  1.00 82.28
ATOM    447  OE2 GLU  61      42.442  17.156   3.458  1.00 82.68
ATOM    448  C   GLU  61      41.083  19.969   7.194  1.00 77.00
ATOM    449  O   GLU  61      41.942  20.327   6.389  1.00 77.10
ATOM    450  N   GLY  62      41.177  20.181   8.502  1.00 76.85
ATOM    451  CA  GLY  62      42.344  20.826   9.069  1.00 76.72
ATOM    452  C   GLY  62      42.415  20.539  10.555  1.00 76.65
ATOM    453  O   GLY  62      42.507  19.380  10.969  1.00 76.79
ATOM    454  N   SER  63      42.361  21.594  11.362  1.00 76.25
ATOM    455  CA  SER  63      42.417  21.458  12.814  1.00 75.06
ATOM    456  CB  SER  63      41.401  20.413  13.300  1.00 75.92
ATOM    457  OG  SER  63      41.350  20.363  14.718  1.00 76.69
ATOM    458  C   SER  63      43.818  21.062  13.259  1.00 73.60
ATOM    459  O   SER  63      44.090  19.899  13.561  1.00 73.10
ATOM    460  N   GLU  64      44.705  22.045  13.280  1.00 71.83
ATOM    461  CA  GLU  64      46.071  21.819  13.703  1.00 70.12
ATOM    462  CB  GLU  64      46.996  22.824  13.011  1.00 71.42
ATOM    463  CG  GLU  64      48.464  22.726  13.417  1.00 73.74
ATOM    464  CD  GLU  64      49.014  21.309  13.342  1.00 74.84
ATOM    465  OE1 GLU  64      48.623  20.466  14.187  1.00 75.26
ATOM    466  OE2 GLU  64      49.837  21.041  12.434  1.00 75.45
ATOM    467  C   GLU  64      46.136  21.971  15.221  1.00 67.97
```

Figure 4

	ATOM	468	O	GLU	64	46.775	22.886	15.734	1.00	68.33
	ATOM	469	N	VAL	65	45.448	21.076	15.927	1.00	65.13
	ATOM	470	CA	VAL	65	45.400	21.067	17.391	1.00	62.32
	ATOM	471	CB	VAL	65	45.335	19.621	17.918	1.00	62.48
	ATOM	472	CG1	VAL	65	45.487	19.607	19.430	1.00	62.45
	ATOM	473	CG2	VAL	65	44.011	18.975	17.508	1.00	62.79
	ATOM	474	C	VAL	65	46.587	21.752	18.055	1.00	60.42
	ATOM	475	O	VAL	65	47.703	21.708	17.540	1.00	60.54
	ATOM	476	N	GLY	66	46.354	22.386	19.200	1.00	58.26
	ATOM	477	CA	GLY	66	47.454	23.043	19.888	1.00	55.67
	ATOM	478	C	GLY	66	47.081	24.174	20.823	1.00	53.42
	ATOM	479	O	GLY	66	46.153	24.052	21.615	1.00	54.08
	ATOM	480	N	ASP	67	47.832	25.267	20.739	1.00	51.06
	ATOM	481	CA	ASP	67	47.614	26.460	21.549	1.00	48.67
	ATOM	482	CB	ASP	67	48.617	26.531	22.703	1.00	49.44
	ATOM	483	CG	ASP	67	48.381	25.462	23.751	1.00	49.34
	ATOM	484	OD1	ASP	67	48.201	24.287	23.365	1.00	49.37
	ATOM	485	OD2	ASP	67	48.386	25.791	24.956	1.00	49.62
	ATOM	486	C	ASP	67	47.832	27.634	20.612	1.00	47.26
	ATOM	487	O	ASP	67	48.786	27.635	19.827	1.00	47.44
	ATOM	488	N	PHE	68	46.955	28.632	20.678	1.00	45.41
	ATOM	489	CA	PHE	68	47.075	29.778	19.785	1.00	43.60
	ATOM	490	CB	PHE	68	46.031	29.682	18.667	1.00	41.17
	ATOM	491	CG	PHE	68	46.032	28.361	17.946	1.00	39.29
	ATOM	492	CD1	PHE	68	45.621	27.199	18.592	1.00	38.55
	ATOM	493	CD2	PHE	68	46.468	28.272	16.623	1.00	38.76
	ATOM	494	CE1	PHE	68	45.647	25.966	17.934	1.00	38.24
	ATOM	495	CE2	PHE	68	46.498	27.050	15.959	1.00	37.31
	ATOM	496	CZ	PHE	68	46.086	25.893	16.619	1.00	37.76
	ATOM	497	C	PHE	68	46.918	31.096	20.514	1.00	43.33
	ATOM	498	O	PHE	68	46.395	31.147	21.621	1.00	43.27
	ATOM	499	N	LEU	69	47.386	32.166	19.889	1.00	43.51
	ATOM	500	CA	LEU	69	47.274	33.475	20.497	1.00	44.73
	ATOM	501	CB	LEU	69	48.625	34.197	20.518	1.00	45.26
	ATOM	502	CG	LEU	69	48.781	34.949	21.848	1.00	46.33
	ATOM	503	CD1	LEU	69	49.166	33.928	22.932	1.00	46.09
	ATOM	504	CD2	LEU	69	49.811	36.072	21.748	1.00	45.48
	ATOM	505	C	LEU	69	46.275	34.278	19.681	1.00	45.37
	ATOM	506	O	LEU	69	46.448	34.451	18.470	1.00	45.62
	ATOM	507	N	SER	70	45.228	34.758	20.351	1.00	45.75
	ATOM	508	CA	SER	70	44.177	35.528	19.697	1.00	44.98
	ATOM	509	CB	SER	70	42.794	34.984	20.074	1.00	44.61
	ATOM	510	OG	SER	70	42.697	33.589	19.844	1.00	44.25
	ATOM	511	C	SER	70	44.250	36.978	20.109	1.00	44.92
	ATOM	512	O	SER	70	44.451	37.289	21.277	1.00	44.67
	ATOM	513	N	LEU	71	44.095	37.858	19.130	1.00	45.85
	ATOM	514	CA	LEU	71	44.092	39.294	19.366	1.00	47.27
	ATOM	515	CB	LEU	71	45.064	40.000	18.421	1.00	47.71
	ATOM	516	CG	LEU	71	46.552	39.942	18.787	1.00	49.06
	ATOM	517	CD1	LEU	71	47.008	38.497	19.039	1.00	49.69
	ATOM	518	CD2	LEU	71	47.348	40.572	17.656	1.00	49.35
	ATOM	519	C	LEU	71	42.668	39.752	19.082	1.00	47.94
	ATOM	520	O	LEU	71	41.873	38.997	18.499	1.00	48.06
	ATOM	521	N	ASP	72	42.333	40.976	19.479	1.00	48.20
	ATOM	522	CA	ASP	72	40.985	41.451	19.244	1.00	48.67
	ATOM	523	CB	ASP	72	40.043	40.807	20.262	1.00	48.71
	ATOM	524	CG	ASP	72	38.668	41.420	20.243	1.00	49.13
	ATOM	525	OD1	ASP	72	38.090	41.549	19.144	1.00	49.57
	ATOM	526	OD2	ASP	72	38.168	41.777	21.331	1.00	50.11

Figure 4

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ATOM    527  C   ASP    72      40.819  42.962  19.258  1.00 48.98
ATOM    528  O   ASP    72      40.247  43.530  20.187  1.00 48.82
ATOM    529  N   LEU    73      41.312  43.613  18.214  1.00 49.73
ATOM    530  CA  LEU    73      41.193  45.060  18.117  1.00 51.48
ATOM    531  CB  LEU    73      42.199  45.603  17.096  1.00 50.80
ATOM    532  CG  LEU    73      42.160  47.096  16.774  1.00 50.07
ATOM    533  CD1 LEU    73      42.358  47.902  18.045  1.00 50.10
ATOM    534  CD2 LEU    73      43.223  47.421  15.738  1.00 49.97
ATOM    535  C   LEU    73      39.764  45.392  17.687  1.00 52.93
ATOM    536  O   LEU    73      38.909  44.507  17.628  1.00 52.38
ATOM    537  N   GLY    74      39.504  46.665  17.401  1.00 54.88
ATOM    538  CA  GLY    74      38.177  47.068  16.983  1.00 56.88
ATOM    539  C   GLY    74      37.285  47.420  18.148  1.00 58.48
ATOM    540  O   GLY    74      36.476  48.348  18.071  1.00 58.31
ATOM    541  N   GLY    75      37.428  46.668  19.233  1.00 60.27
ATOM    542  CA  GLY    75      36.621  46.925  20.410  1.00 62.46
ATOM    543  C   GLY    75      37.020  48.230  21.074  1.00 63.75
ATOM    544  O   GLY    75      37.824  49.005  20.536  1.00 64.06
ATOM    545  N   THR    76      36.452  48.481  22.248  1.00 64.50
ATOM    546  CA  THR    76      36.759  49.697  22.991  1.00 65.42
ATOM    547  CB  THR    76      35.905  49.776  24.266  1.00 66.28
ATOM    548  OG1 THR    76      36.361  48.791  25.203  1.00 67.43
ATOM    549  CG2 THR    76      34.425  49.505  23.938  1.00 66.14
ATOM    550  C   THR    76      38.238  49.651  23.385  1.00 65.25
ATOM    551  O   THR    76      39.005  50.595  23.152  1.00 65.01
ATOM    552  N   ASN    77      38.622  48.528  23.980  1.00 64.74
ATOM    553  CA  ASN    77      39.987  48.309  24.412  1.00 64.17
ATOM    554  CB  ASN    77      40.015  47.966  25.903  1.00 65.44
ATOM    555  CG  ASN    77      39.346  49.027  26.765  1.00 66.47
ATOM    556  OD1 ASN    77      39.656  50.219  26.663  1.00 67.13
ATOM    557  ND2 ASN    77      38.431  48.596  27.629  1.00 66.65
ATOM    558  C   ASN    77      40.547  47.149  23.603  1.00 63.19
ATOM    559  O   ASN    77      39.795  46.303  23.120  1.00 62.58
ATOM    560  N   PHE    78      41.866  47.123  23.446  1.00 62.14
ATOM    561  CA  PHE    78      42.526  46.051  22.708  1.00 61.12
ATOM    562  CB  PHE    78      43.887  46.514  22.172  1.00 61.81
ATOM    563  CG  PHE    78      44.684  45.420  21.516  1.00 62.50
ATOM    564  CD1 PHE    78      44.347  44.956  20.245  1.00 62.81
ATOM    565  CD2 PHE    78      45.741  44.818  22.189  1.00 62.99
ATOM    566  CE1 PHE    78      45.051  43.899  19.655  1.00 62.72
ATOM    567  CE2 PHE    78      46.450  43.763  21.607  1.00 63.38
ATOM    568  CZ  PHE    78      46.103  43.301  20.336  1.00 63.01
ATOM    569  C   PHE    78      42.732  44.893  23.668  1.00 60.09
ATOM    570  O   PHE    78      43.065  45.100  24.834  1.00 60.08
ATOM    571  N   ARG    79      42.528  43.675  23.184  1.00 58.63
ATOM    572  CA  ARG    79      42.706  42.504  24.025  1.00 57.40
ATOM    573  CB  ARG    79      41.367  41.819  24.280  1.00 57.06
ATOM    574  CG  ARG    79      41.481  40.637  25.222  1.00 57.49
ATOM    575  CD  ARG    79      40.221  39.819  25.219  1.00 57.47
ATOM    576  NE  ARG    79      39.062  40.646  25.504  1.00 57.16
ATOM    577  CZ  ARG    79      37.818  40.266  25.267  1.00 57.69
ATOM    578  NH1 ARG    79      37.586  39.071  24.738  1.00 57.38
ATOM    579  NH2 ARG    79      36.812  41.080  25.555  1.00 58.45
ATOM    580  C   ARG    79      43.663  41.522  23.368  1.00 56.71
ATOM    581  O   ARG    79      43.926  41.619  22.170  1.00 57.24
ATOM    582  N   VAL    80      44.180  40.590  24.167  1.00 55.50
ATOM    583  CA  VAL    80      45.114  39.557  23.724  1.00 54.27
ATOM    584  CB  VAL    80      46.576  39.947  23.996  1.00 54.31
ATOM    585  CG1 VAL    80      47.491  38.779  23.674  1.00 54.49
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Figure 4

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ATOM    586  CG2 VAL    80      46.960  41.158  23.166  1.00 54.39
ATOM    587  C   VAL    80      44.806  38.327  24.555  1.00 54.04
ATOM    588  O   VAL    80      44.517  38.447  25.738  1.00 53.31
ATOM    589  N   MSE    81      44.881  37.144  23.957  1.00 54.52
ATOM    590  CA  MSE    81      44.568  35.935  24.703  1.00 54.59
ATOM    591  CB  MSE    81      43.053  35.804  24.828  1.00 57.08
ATOM    592  CG  MSE    81      42.300  36.025  23.520  1.00 60.39
ATOM    593  SE  MSE    81      40.534  36.437  23.792  1.00 65.62
ATOM    594  CE  MSE    81      39.999  34.926  24.679  1.00 62.03
ATOM    595  C   MSE    81      45.142  34.645  24.146  1.00 53.56
ATOM    596  O   MSE    81      45.598  34.582  23.007  1.00 52.99
ATOM    597  N   LEU    82      45.096  33.611  24.978  1.00 52.63
ATOM    598  CA  LEU    82      45.602  32.292  24.638  1.00 51.86
ATOM    599  CB  LEU    82      46.660  31.863  25.665  1.00 52.75
ATOM    600  CG  LEU    82      47.261  30.455  25.542  1.00 53.22
ATOM    601  CD1 LEU    82      48.562  30.521  24.736  1.00 52.42
ATOM    602  CD2 LEU    82      47.523  29.882  26.937  1.00 53.00
ATOM    603  C   LEU    82      44.461  31.286  24.650  1.00 51.18
ATOM    604  O   LEU    82      43.718  31.186  25.632  1.00 51.20
ATOM    605  N   VAL    83      44.333  30.535  23.563  1.00 50.58
ATOM    606  CA  VAL    83      43.292  29.522  23.448  1.00 50.00
ATOM    607  CB  VAL    83      42.274  29.887  22.362  1.00 49.63
ATOM    608  CG1 VAL    83      41.213  28.794  22.262  1.00 49.26
ATOM    609  CG2 VAL    83      41.660  31.244  22.670  1.00 48.32
ATOM    610  C   VAL    83      43.914  28.187  23.080  1.00 50.53
ATOM    611  O   VAL    83      44.759  28.122  22.192  1.00 50.93
ATOM    612  N   LYS    84      43.496  27.127  23.763  1.00 51.05
ATOM    613  CA  LYS    84      44.017  25.788  23.504  1.00 51.89
ATOM    614  CB  LYS    84      44.338  25.061  24.826  1.00 51.79
ATOM    615  CG  LYS    84      44.716  23.581  24.659  1.00 51.85
ATOM    616  CD  LYS    84      44.951  22.870  26.009  1.00 51.58
ATOM    617  CE  LYS    84      46.429  22.848  26.422  1.00 50.92
ATOM    618  NZ  LYS    84      47.041  24.198  26.592  1.00 50.33
ATOM    619  C   LYS    84      42.997  24.983  22.708  1.00 52.68
ATOM    620  O   LYS    84      42.115  24.327  23.282  1.00 53.00
ATOM    621  N   VAL    85      43.124  25.038  21.383  1.00 52.91
ATOM    622  CA  VAL    85      42.224  24.319  20.488  1.00 52.70
ATOM    623  CB  VAL    85      42.399  24.805  19.048  1.00 51.79
ATOM    624  CG1 VAL    85      41.302  24.232  18.176  1.00 52.19
ATOM    625  CG2 VAL    85      42.389  26.319  19.017  1.00 51.59
ATOM    626  C   VAL    85      42.525  22.823  20.548  1.00 53.51
ATOM    627  O   VAL    85      43.637  22.389  20.243  1.00 53.87
ATOM    628  N   GLY    86      41.534  22.037  20.952  1.00 54.38
ATOM    629  CA  GLY    86      41.726  20.603  21.053  1.00 55.35
ATOM    630  C   GLY    86      40.901  19.810  20.060  1.00 56.21
ATOM    631  O   GLY    86      40.136  20.370  19.278  1.00 55.63
ATOM    632  N   GLU    87      41.050  18.493  20.106  1.00 57.81
ATOM    633  CA  GLU    87      40.339  17.611  19.195  1.00 59.64
ATOM    634  CB  GLU    87      41.290  16.529  18.673  1.00 60.88
ATOM    635  CG  GLU    87      40.680  15.648  17.611  1.00 62.26
ATOM    636  CD  GLU    87      40.215  16.457  16.423  1.00 63.21
ATOM    637  OE1 GLU    87      41.072  16.931  15.644  1.00 63.20
ATOM    638  OE2 GLU    87      38.989  16.631  16.278  1.00 64.58
ATOM    639  C   GLU    87      39.133  16.959  19.859  1.00 60.12
ATOM    640  O   GLU    87      39.271  16.187  20.810  1.00 60.00
ATOM    641  N   GLY    88      37.948  17.273  19.347  1.00 60.93
ATOM    642  CA  GLY    88      36.735  16.707  19.902  1.00 61.61
ATOM    643  C   GLY    88      35.840  16.120  18.833  1.00 62.11
ATOM    644  O   GLY    88      36.038  16.346  17.638  1.00 61.67
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Figure 4

	ATOM	645	N	GLU	89	34.845	15.363	19.274	1.00	62.79
	ATOM	646	CA	GLU	89	33.898	14.724	18.372	1.00	63.90
	ATOM	647	CB	GLU	89	32.782	14.089	19.203	1.00	63.50
	ATOM	648	CG	GLU	89	33.304	13.137	20.275	1.00	62.64
5	ATOM	649	CD	GLU	89	32.214	12.623	21.203	1.00	62.46
	ATOM	650	OE1	GLU	89	32.510	11.728	22.019	1.00	62.39
	ATOM	651	OE2	GLU	89	31.064	13.110	21.128	1.00	62.11
	ATOM	652	C	GLU	89	33.312	15.688	17.325	1.00	65.16
	ATOM	653	O	GLU	89	32.975	16.837	17.634	1.00	64.98
10	ATOM	654	N	GLU	90	33.204	15.205	16.087	1.00	66.03
	ATOM	655	CA	GLU	90	32.667	15.977	14.958	1.00	66.67
	ATOM	656	CB	GLU	90	31.135	15.974	14.978	1.00	67.21
	ATOM	657	CG	GLU	90	30.495	14.620	14.717	1.00	66.83
	ATOM	658	CD	GLU	90	28.986	14.662	14.869	1.00	67.49
15	ATOM	659	OE1	GLU	90	28.308	15.273	14.009	1.00	67.17
	ATOM	660	OE2	GLU	90	28.480	14.090	15.858	1.00	66.84
	ATOM	661	C	GLU	90	33.149	17.421	14.871	1.00	66.91
	ATOM	662	O	GLU	90	32.623	18.212	14.080	1.00	66.74
	ATOM	663	N	GLY	91	34.149	17.769	15.671	1.00	67.05
20	ATOM	664	CA	GLY	91	34.649	19.126	15.628	1.00	67.38
	ATOM	665	C	GLY	91	36.036	19.339	16.201	1.00	67.42
	ATOM	666	O	GLY	91	37.025	18.797	15.708	1.00	68.24
	ATOM	667	N	GLN	92	36.094	20.154	17.246	1.00	66.86
	ATOM	668	CA	GLN	92	37.335	20.492	17.929	1.00	65.93
25	ATOM	669	CB	GLN	92	38.395	20.968	16.924	1.00	66.17
	ATOM	670	CG	GLN	92	38.007	22.215	16.159	1.00	66.24
	ATOM	671	CD	GLN	92	38.564	22.236	14.750	1.00	66.57
	ATOM	672	OE1	GLN	92	38.432	21.260	14.007	1.00	66.37
	ATOM	673	NE2	GLN	92	39.177	23.356	14.367	1.00	66.54
30	ATOM	674	C	GLN	92	36.999	21.605	18.920	1.00	65.21
	ATOM	675	O	GLN	92	36.625	22.721	18.530	1.00	65.44
	ATOM	676	N	TRP	93	37.111	21.278	20.204	1.00	63.62
	ATOM	677	CA	TRP	93	36.820	22.227	21.261	1.00	61.61
	ATOM	678	CB	TRP	93	36.859	21.540	22.626	1.00	62.77
35	ATOM	679	CG	TRP	93	38.050	20.641	22.857	1.00	63.86
	ATOM	680	CD2	TRP	93	39.213	20.943	23.637	1.00	64.17
	ATOM	681	CE2	TRP	93	40.026	19.787	23.645	1.00	64.21
	ATOM	682	CE3	TRP	93	39.647	22.080	24.336	1.00	64.11
	ATOM	683	CD1	TRP	93	38.206	19.349	22.424	1.00	63.84
40	ATOM	684	NE1	TRP	93	39.387	18.830	22.897	1.00	63.69
	ATOM	685	CZ2	TRP	93	41.246	19.731	24.324	1.00	64.43
	ATOM	686	CZ3	TRP	93	40.859	22.026	25.009	1.00	64.63
	ATOM	687	CH2	TRP	93	41.645	20.857	24.999	1.00	64.71
	ATOM	688	C	TRP	93	37.784	23.393	21.248	1.00	59.53
45	ATOM	689	O	TRP	93	38.733	23.420	20.474	1.00	59.18
	ATOM	690	N	SER	94	37.521	24.366	22.106	1.00	57.94
	ATOM	691	CA	SER	94	38.353	25.549	22.207	1.00	56.46
	ATOM	692	CB	SER	94	37.880	26.615	21.219	1.00	56.58
	ATOM	693	OG	SER	94	36.504	26.899	21.412	1.00	56.78
50	ATOM	694	C	SER	94	38.185	26.050	23.624	1.00	55.56
	ATOM	695	O	SER	94	37.142	25.822	24.237	1.00	55.36
	ATOM	696	N	VAL	95	39.208	26.722	24.146	1.00	54.53
	ATOM	697	CA	VAL	95	39.152	27.248	25.504	1.00	53.17
	ATOM	698	CB	VAL	95	39.511	26.183	26.549	1.00	52.17
55	ATOM	699	CG1	VAL	95	39.742	26.844	27.891	1.00	52.13
	ATOM	700	CG2	VAL	95	38.396	25.172	26.666	1.00	51.73
	ATOM	701	C	VAL	95	40.099	28.399	25.719	1.00	52.74
	ATOM	702	O	VAL	95	41.268	28.315	25.357	1.00	53.14
	ATOM	703	N	LYS	96	39.587	29.469	26.318	1.00	52.63

Figure 4

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ATOM    704  CA  LYS    96      40.402  30.637  26.629  1.00 52.93
ATOM    705  CB  LYS    96      39.513  31.849  26.932  1.00 53.25
ATOM    706  CG  LYS    96      40.277  33.129  27.231  1.00 53.79
ATOM    707  CD  LYS    96      39.910  33.706  28.595  1.00 54.80
ATOM    708  CE  LYS    96      38.427  34.102  28.682  1.00 55.69
ATOM    709  NZ  LYS    96      38.027  35.162  27.696  1.00 55.59
ATOM    710  C   LYS    96      41.154  30.218  27.882  1.00 52.96
ATOM    711  O   LYS    96      40.546  29.733  28.834  1.00 52.93
ATOM    712  N   THR    97      42.470  30.384  27.886  1.00 53.38
ATOM    713  CA  THR    97      43.253  29.980  29.050  1.00 53.93
ATOM    714  CB  THR    97      44.238  28.850  28.684  1.00 53.99
ATOM    715  OG1 THR    97      43.512  27.736  28.151  1.00 52.99
ATOM    716  CG2 THR    97      44.998  28.394  29.918  1.00 55.29
ATOM    717  C   THR    97      44.036  31.132  29.670  1.00 53.82
ATOM    718  O   THR    97      44.330  31.123  30.866  1.00 53.94
ATOM    719  N   LYS    98      44.373  32.117  28.848  1.00 53.85
ATOM    720  CA  LYS    98      45.115  33.276  29.315  1.00 54.60
ATOM    721  CB  LYS    98      46.627  33.096  29.087  1.00 55.51
ATOM    722  CG  LYS    98      47.220  31.809  29.652  1.00 56.78
ATOM    723  CD  LYS    98      47.074  31.733  31.162  1.00 58.23
ATOM    724  CE  LYS    98      47.553  30.389  31.713  1.00 58.82
ATOM    725  NZ  LYS    98      47.404  30.320  33.201  1.00 58.98
ATOM    726  C   LYS    98      44.644  34.479  28.518  1.00 54.54
ATOM    727  O   LYS    98      44.323  34.360  27.329  1.00 54.79
ATOM    728  N   HIS    99      44.590  35.632  29.173  1.00 54.03
ATOM    729  CA  HIS    99      44.193  36.853  28.496  1.00 54.03
ATOM    730  CB  HIS    99      42.720  36.793  28.052  1.00 55.02
ATOM    731  CG  HIS    99      41.732  36.872  29.172  1.00 55.71
ATOM    732  CD2 HIS    99      40.682  37.704  29.373  1.00 55.66
ATOM    733  ND1 HIS    99      41.739  35.999  30.239  1.00 56.19
ATOM    734  CE1 HIS    99      40.736  36.288  31.049  1.00 56.30
ATOM    735  NE2 HIS    99      40.080  37.319  30.546  1.00 56.72
ATOM    736  C   HIS    99      44.445  38.082  29.351  1.00 53.46
ATOM    737  O   HIS    99      44.526  38.007  30.577  1.00 53.47
ATOM    738  N   GLN   100      44.583  39.214  28.683  1.00 52.94
ATOM    739  CA  GLN   100      44.841  40.468  29.349  1.00 53.34
ATOM    740  CB  GLN   100      46.354  40.649  29.513  1.00 53.39
ATOM    741  CG  GLN   100      46.790  42.001  30.055  1.00 54.26
ATOM    742  CD  GLN   100      46.168  42.345  31.394  1.00 54.43
ATOM    743  OE1 GLN   100      46.349  41.629  32.384  1.00 55.27
ATOM    744  NE2 GLN   100      45.433  43.452  31.432  1.00 53.60
ATOM    745  C   GLN   100      44.243  41.567  28.481  1.00 53.43
ATOM    746  O   GLN   100      44.416  41.569  27.260  1.00 53.75
ATOM    747  N   THR   101      43.527  42.493  29.105  1.00 52.90
ATOM    748  CA  THR   101      42.905  43.576  28.367  1.00 53.12
ATOM    749  CB  THR   101      41.495  43.826  28.894  1.00 52.52
ATOM    750  OG1 THR   101      40.789  42.582  28.925  1.00 52.85
ATOM    751  CG2 THR   101      40.752  44.808  27.999  1.00 52.23
ATOM    752  C   THR   101      43.731  44.845  28.499  1.00 53.61
ATOM    753  O   THR   101      44.285  45.108  29.563  1.00 53.95
ATOM    754  N   TYR   102      43.809  45.628  27.422  1.00 54.10
ATOM    755  CA  TYR   102      44.585  46.869  27.422  1.00 55.36
ATOM    756  CB  TYR   102      45.878  46.708  26.608  1.00 54.89
ATOM    757  CG  TYR   102      46.788  45.569  27.015  1.00 54.25
ATOM    758  CD1 TYR   102      46.382  44.241  26.888  1.00 54.08
ATOM    759  CE1 TYR   102      47.227  43.197  27.226  1.00 53.44
ATOM    760  CD2 TYR   102      48.069  45.822  27.497  1.00 53.79
ATOM    761  CE2 TYR   102      48.922  44.785  27.840  1.00 53.76
ATOM    762  CZ  TYR   102      48.498  43.475  27.701  1.00 53.85
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Figure 4

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ATOM    763  OH  TYR   102      49.355  42.442  28.021  1.00 54.03
ATOM    764  C   TYR   102      43.813  48.041  26.822  1.00 56.65
ATOM    765  O   TYR   102      43.173  47.899  25.781  1.00 56.91
ATOM    766  N   SER   103      43.891  49.203  27.462  1.00 58.50
ATOM    767  CA  SER   103      43.217  50.385  26.938  1.00 60.94
ATOM    768  CB  SER   103      42.997  51.411  28.049  1.00 61.09
ATOM    769  OG  SER   103      44.231  51.829  28.602  1.00 62.50
ATOM    770  C   SER   103      44.090  50.985  25.833  1.00 62.31
ATOM    771  O   SER   103      45.293  50.729  25.771  1.00 62.27
ATOM    772  N   ALA   104      43.487  51.783  24.960  1.00 64.47
ATOM    773  CA  ALA   104      44.226  52.386  23.856  1.00 67.01
ATOM    774  CB  ALA   104      43.516  52.093  22.526  1.00 67.01
ATOM    775  C   ALA   104      44.410  53.888  24.025  1.00 68.66
ATOM    776  O   ALA   104      43.458  54.658  23.902  1.00 69.01
ATOM    777  N   PRO   105      45.648  54.327  24.305  1.00 70.09
ATOM    778  CD  PRO   105      46.878  53.522  24.397  1.00 70.06
ATOM    779  CA  PRO   105      45.946  55.751  24.485  1.00 71.25
ATOM    780  CB  PRO   105      47.443  55.748  24.783  1.00 70.79
ATOM    781  CG  PRO   105      47.929  54.535  24.046  1.00 70.54
ATOM    782  C   PRO   105      45.592  56.586  23.251  1.00 72.81
ATOM    783  O   PRO   105      45.837  56.170  22.117  1.00 73.09
ATOM    784  N   GLU   106      45.012  57.762  23.479  1.00 74.39
ATOM    785  CA  GLU   106      44.619  58.652  22.391  1.00 76.25
ATOM    786  CB  GLU   106      43.991  59.921  22.950  1.00 76.77
ATOM    787  CG  GLU   106      42.702  59.673  23.680  1.00 78.35
ATOM    788  CD  GLU   106      42.397  60.775  24.657  1.00 79.28
ATOM    789  OE1 GLU   106      42.239  61.934  24.214  1.00 79.74
ATOM    790  OE2 GLU   106      42.326  60.478  25.871  1.00 80.03
ATOM    791  C   GLU   106      45.784  59.028  21.494  1.00 77.33
ATOM    792  O   GLU   106      45.600  59.262  20.300  1.00 77.48
ATOM    793  N   ASP   107      46.980  59.104  22.068  1.00 78.72
ATOM    794  CA  ASP   107      48.161  59.440  21.284  1.00 80.10
ATOM    795  CB  ASP   107      49.431  59.316  22.134  1.00 80.44
ATOM    796  CG  ASP   107      49.965  57.889  22.185  1.00 81.03
ATOM    797  OD1 ASP   107      49.198  56.976  22.569  1.00 81.42
ATOM    798  OD2 ASP   107      51.151  57.682  21.839  1.00 80.86
ATOM    799  C   ASP   107      48.212  58.424  20.151  1.00 80.92
ATOM    800  O   ASP   107      48.724  58.703  19.065  1.00 81.29
ATOM    801  N   ALA   108      47.670  57.241  20.428  1.00 81.68
ATOM    802  CA  ALA   108      47.628  56.151  19.463  1.00 82.45
ATOM    803  CB  ALA   108      47.605  54.813  20.200  1.00 82.45
ATOM    804  C   ALA   108      46.406  56.275  18.553  1.00 82.91
ATOM    805  O   ALA   108      46.536  56.351  17.331  1.00 82.98
ATOM    806  N   MSE   109      45.221  56.303  19.157  1.00 83.41
ATOM    807  CA  MSE   109      43.974  56.414  18.407  1.00 83.78
ATOM    808  CB  MSE   109      42.787  56.519  19.368  1.00 85.45
ATOM    809  CG  MSE   109      41.581  55.678  18.972  1.00 87.01
ATOM    810  SE  MSE   109      41.933  53.898  19.096  1.00 90.12
ATOM    811  CE  MSE   109      42.665  53.581  17.453  1.00 88.95
ATOM    812  C   MSE   109      43.992  57.633  17.494  1.00 83.17
ATOM    813  O   MSE   109      43.235  57.710  16.527  1.00 83.19
ATOM    814  N   THR   110      44.854  58.590  17.820  1.00 82.51
ATOM    815  CA  THR   110      44.986  59.815  17.040  1.00 82.00
ATOM    816  CB  THR   110      45.289  61.022  17.949  1.00 82.44
ATOM    817  OG1 THR   110      44.302  61.103  18.986  1.00 83.00
ATOM    818  CG2 THR   110      45.283  62.313  17.142  1.00 82.69
ATOM    819  C   THR   110      46.150  59.640  16.082  1.00 81.25
ATOM    820  O   THR   110      46.127  60.123  14.949  1.00 80.95
ATOM    821  N   GLY   111      47.168  58.933  16.559  1.00 80.84
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Figure 4

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ATOM    822  CA  GLY  111      48.358  58.691  15.768  1.00 80.12
ATOM    823  C   GLY  111      48.121  57.986  14.450  1.00 79.53
ATOM    824  O   GLY  111      47.018  57.531  14.148  1.00 79.54
ATOM    825  N   THR  112      49.181  57.904  13.658  1.00 78.87
ATOM    826  CA  THR  112      49.129  57.254  12.360  1.00 78.09
ATOM    827  CB  THR  112      50.427  57.553  11.561  1.00 78.67
ATOM    828  OG1 THR  112      50.329  57.001  10.240  1.00 79.18
ATOM    829  CG2 THR  112      51.644  56.956  12.279  1.00 78.48
ATOM    830  C   THR  112      48.992  55.748  12.579  1.00 77.09
ATOM    831  O   THR  112      49.231  55.254  13.685  1.00 76.48
ATOM    832  N   ALA  113      48.601  55.027  11.529  1.00 76.26
ATOM    833  CA  ALA  113      48.443  53.573  11.603  1.00 75.60
ATOM    834  CB  ALA  113      48.184  53.001  10.208  1.00 76.00
ATOM    835  C   ALA  113      49.711  52.965  12.191  1.00 74.65
ATOM    836  O   ALA  113      49.665  52.006  12.968  1.00 74.58
ATOM    837  N   GLU  114      50.845  53.538  11.803  1.00 73.24
ATOM    838  CA  GLU  114      52.139  53.088  12.288  1.00 71.57
ATOM    839  CB  GLU  114      53.246  53.971  11.700  1.00 72.34
ATOM    840  CG  GLU  114      53.130  54.167  10.188  1.00 71.64
ATOM    841  CD  GLU  114      53.325  52.877   9.401  1.00 72.49
ATOM    842  OE1 GLU  114      53.192  51.781   9.994  1.00 72.24
ATOM    843  OE2 GLU  114      53.600  52.960   8.183  1.00 71.83
ATOM    844  C   GLU  114      52.085  53.233  13.801  1.00 70.37
ATOM    845  O   GLU  114      52.297  52.266  14.537  1.00 69.92
ATOM    846  N   MET  115      51.778  54.450  14.246  1.00 68.75
ATOM    847  CA  MET  115      51.657  54.760  15.669  1.00 66.97
ATOM    848  CB  MET  115      51.013  56.140  15.866  1.00 67.15
ATOM    849  CG  MET  115      51.999  57.277  16.040  1.00 66.94
ATOM    850  SD  MET  115      53.203  56.869  17.320  1.00 67.61
ATOM    851  CE  MET  115      52.137  56.732  18.788  1.00 66.65
ATOM    852  C   MET  115      50.799  53.718  16.374  1.00 65.81
ATOM    853  O   MET  115      51.266  53.010  17.275  1.00 65.94
ATOM    854  N   LEU  116      49.542  53.635  15.940  1.00 63.70
ATOM    855  CA  LEU  116      48.561  52.711  16.504  1.00 61.63
ATOM    856  CB  LEU  116      47.287  52.720  15.650  1.00 60.89
ATOM    857  CG  LEU  116      45.948  52.226  16.205  1.00 59.42
ATOM    858  CD1 LEU  116      44.953  52.182  15.051  1.00 58.84
ATOM    859  CD2 LEU  116      46.081  50.858  16.847  1.00 58.86
ATOM    860  C   LEU  116      49.083  51.285  16.613  1.00 60.35
ATOM    861  O   LEU  116      48.977  50.665  17.667  1.00 60.48
ATOM    862  N   PHE  117      49.641  50.756  15.531  1.00 59.14
ATOM    863  CA  PHE  117      50.138  49.391  15.580  1.00 58.14
ATOM    864  CB  PHE  117      50.298  48.819  14.173  1.00 57.03
ATOM    865  CG  PHE  117      49.055  48.144  13.669  1.00 56.22
ATOM    866  CD1 PHE  117      48.005  48.889  13.143  1.00 55.49
ATOM    867  CD2 PHE  117      48.909  46.763  13.783  1.00 55.59
ATOM    868  CE1 PHE  117      46.830  48.270  12.741  1.00 55.25
ATOM    869  CE2 PHE  117      47.736  46.134  13.384  1.00 55.20
ATOM    870  CZ  PHE  117      46.695  46.887  12.862  1.00 55.23
ATOM    871  C   PHE  117      51.415  49.204  16.382  1.00 57.89
ATOM    872  O   PHE  117      51.799  48.073  16.690  1.00 57.80
ATOM    873  N   ALA  118      52.078  50.303  16.725  1.00 57.35
ATOM    874  CA  ALA  118      53.275  50.193  17.537  1.00 56.79
ATOM    875  CB  ALA  118      54.004  51.533  17.594  1.00 56.42
ATOM    876  C   ALA  118      52.747  49.792  18.922  1.00 56.46
ATOM    877  O   ALA  118      53.220  48.829  19.536  1.00 56.68
ATOM    878  N   ALA  119      51.733  50.515  19.391  1.00 55.57
ATOM    879  CA  ALA  119      51.142  50.226  20.693  1.00 55.05
ATOM    880  CB  ALA  119      49.931  51.135  20.952  1.00 53.91
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Figure 4

ATOM	881	C	ALA	119	50.719	48.769	20.763	1.00	54.96
ATOM	882	O	ALA	119	51.090	48.052	21.698	1.00	54.94
ATOM	883	N	ILE	120	49.948	48.338	19.763	1.00	55.10
ATOM	884	CA	ILE	120	49.443	46.969	19.715	1.00	55.51
ATOM	885	CB	ILE	120	48.679	46.679	18.397	1.00	54.45
ATOM	886	CG2	ILE	120	47.922	45.363	18.525	1.00	53.30
ATOM	887	CG1	ILE	120	47.688	47.808	18.089	1.00	53.32
ATOM	888	CD1	ILE	120	46.871	47.581	16.820	1.00	51.70
ATOM	889	C	ILE	120	50.575	45.957	19.846	1.00	56.57
ATOM	890	O	ILE	120	50.477	45.006	20.632	1.00	56.52
ATOM	891	N	SER	121	51.645	46.169	19.076	1.00	57.78
ATOM	892	CA	SER	121	52.814	45.284	19.093	1.00	58.54
ATOM	893	CB	SER	121	53.844	45.730	18.045	1.00	58.96
ATOM	894	OG	SER	121	53.377	45.507	16.720	1.00	59.32
ATOM	895	C	SER	121	53.457	45.280	20.473	1.00	58.74
ATOM	896	O	SER	121	54.007	44.265	20.918	1.00	57.56
ATOM	897	N	GLU	122	53.379	46.422	21.151	1.00	59.50
ATOM	898	CA	GLU	122	53.947	46.529	22.484	1.00	60.44
ATOM	899	CB	GLU	122	54.003	47.986	22.941	1.00	60.60
ATOM	900	CG	GLU	122	55.104	48.241	23.952	1.00	60.45
ATOM	901	CD	GLU	122	54.706	49.252	25.003	1.00	61.76
ATOM	902	OE1	GLU	122	54.152	50.312	24.630	1.00	61.92
ATOM	903	OE2	GLU	122	54.950	48.986	26.202	1.00	62.20
ATOM	904	C	GLU	122	53.091	45.725	23.452	1.00	60.63
ATOM	905	O	GLU	122	53.565	44.761	24.048	1.00	60.82
ATOM	906	N	CYS	123	51.831	46.120	23.605	1.00	60.96
ATOM	907	CA	CYS	123	50.936	45.410	24.510	1.00	61.79
ATOM	908	CB	CYS	123	49.481	45.840	24.278	1.00	61.63
ATOM	909	SG	CYS	123	49.191	47.636	24.439	1.00	62.83
ATOM	910	C	CYS	123	51.107	43.922	24.233	1.00	61.90
ATOM	911	O	CYS	123	51.028	43.095	25.147	1.00	61.89
ATOM	912	N	ILE	124	51.350	43.588	22.966	1.00	62.36
ATOM	913	CA	ILE	124	51.561	42.197	22.588	1.00	62.79
ATOM	914	CB	ILE	124	52.033	42.061	21.109	1.00	62.52
ATOM	915	CG2	ILE	124	52.618	40.676	20.877	1.00	61.07
ATOM	916	CG1	ILE	124	50.866	42.280	20.138	1.00	61.53
ATOM	917	CD1	ILE	124	50.016	41.038	19.888	1.00	61.77
ATOM	918	C	ILE	124	52.673	41.706	23.499	1.00	62.76
ATOM	919	O	ILE	124	52.475	40.807	24.320	1.00	62.23
ATOM	920	N	SER	125	53.839	42.327	23.347	1.00	63.43
ATOM	921	CA	SER	125	55.020	42.002	24.138	1.00	64.63
ATOM	922	CB	SER	125	56.062	43.117	23.986	1.00	65.05
ATOM	923	OG	SER	125	57.324	42.745	24.523	1.00	67.01
ATOM	924	C	SER	125	54.646	41.840	25.610	1.00	64.32
ATOM	925	O	SER	125	54.886	40.794	26.219	1.00	64.46
ATOM	926	N	ASP	126	54.047	42.884	26.169	1.00	64.43
ATOM	927	CA	ASP	126	53.626	42.894	27.562	1.00	64.86
ATOM	928	CB	ASP	126	52.660	44.060	27.788	1.00	64.95
ATOM	929	CG	ASP	126	52.390	44.323	29.253	1.00	65.38
ATOM	930	OD1	ASP	126	51.952	43.389	29.955	1.00	65.74
ATOM	931	OD2	ASP	126	52.613	45.467	29.706	1.00	65.92
ATOM	932	C	ASP	126	52.968	41.572	27.980	1.00	64.65
ATOM	933	O	ASP	126	53.424	40.918	28.924	1.00	64.28
ATOM	934	N	PHE	127	51.902	41.189	27.274	1.00	64.96
ATOM	935	CA	PHE	127	51.177	39.948	27.565	1.00	65.21
ATOM	936	CB	PHE	127	50.145	39.657	26.468	1.00	64.22
ATOM	937	CG	PHE	127	49.569	38.258	26.525	1.00	63.67
ATOM	938	CD1	PHE	127	48.774	37.857	27.594	1.00	63.64
ATOM	939	CD2	PHE	127	49.830	37.343	25.512	1.00	63.42

Figure 4

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ATOM    940  CE1 PHE   127      48.247  36.564  27.652  1.00 63.40
ATOM    941  CE2 PHE   127      49.308  36.051  25.560  1.00 63.55
ATOM    942  CZ  PHE   127      48.516  35.661  26.632  1.00 63.49
ATOM    943  C   PHE   127      52.154  38.791  27.631  1.00 65.83
ATOM    944  O   PHE   127      52.195  38.030  28.600  1.00 65.71
ATOM    945  N   LEU   128      52.931  38.684  26.562  1.00 66.57
ATOM    946  CA  LEU   128      53.942  37.656  26.387  1.00 67.52
ATOM    947  CB  LEU   128      54.773  38.022  25.166  1.00 67.64
ATOM    948  CG  LEU   128      53.926  38.452  23.969  1.00 67.42
ATOM    949  CD1 LEU   128      54.819  39.108  22.941  1.00 67.90
ATOM    950  CD2 LEU   128      53.195  37.251  23.387  1.00 67.65
ATOM    951  C   LEU   128      54.850  37.502  27.609  1.00 68.09
ATOM    952  O   LEU   128      54.829  36.468  28.285  1.00 67.92
ATOM    953  N   ASP   129      55.654  38.530  27.878  1.00 68.62
ATOM    954  CA  ASP   129      56.565  38.514  29.018  1.00 69.22
ATOM    955  CB  ASP   129      57.135  39.907  29.287  1.00 68.93
ATOM    956  CG  ASP   129      58.115  40.342  28.239  1.00 68.90
ATOM    957  OD1 ASP   129      59.100  39.606  28.011  1.00 69.12
ATOM    958  OD2 ASP   129      57.900  41.423  27.650  1.00 69.22
ATOM    959  C   ASP   129      55.843  38.059  30.267  1.00 69.59
ATOM    960  O   ASP   129      56.063  36.956  30.761  1.00 69.41
ATOM    961  N   LYS   130      54.973  38.940  30.753  1.00 70.10
ATOM    962  CA  LYS   130      54.190  38.733  31.958  1.00 70.67
ATOM    963  CB  LYS   130      53.285  39.946  32.159  1.00 70.80
ATOM    964  CG  LYS   130      54.076  41.252  32.052  1.00 70.54
ATOM    965  CD  LYS   130      53.218  42.479  32.266  1.00 70.22
ATOM    966  CE  LYS   130      54.021  43.746  32.011  1.00 70.07
ATOM    967  NZ  LYS   130      53.204  44.977  32.195  1.00 69.69
ATOM    968  C   LYS   130      53.394  37.441  31.982  1.00 71.17
ATOM    969  O   LYS   130      52.381  37.331  32.673  1.00 70.99
ATOM    970  N   HIS   131      53.883  36.468  31.221  1.00 72.01
ATOM    971  CA  HIS   131      53.301  35.139  31.125  1.00 73.44
ATOM    972  CB  HIS   131      52.313  35.065  29.965  1.00 73.00
ATOM    973  CG  HIS   131      50.881  35.076  30.397  1.00 72.93
ATOM    974  CD2 HIS   131      49.960  34.085  30.454  1.00 72.73
ATOM    975  ND1 HIS   131      50.256  36.210  30.869  1.00 72.87
ATOM    976  CE1 HIS   131      49.010  35.917  31.196  1.00 73.01
ATOM    977  NE2 HIS   131      48.806  34.634  30.954  1.00 73.04
ATOM    978  C   HIS   131      54.424  34.124  30.908  1.00 74.61
ATOM    979  O   HIS   131      54.419  33.049  31.514  1.00 74.70
ATOM    980  N   GLN   132      55.374  34.502  30.046  1.00 76.14
ATOM    981  CA  GLN   132      56.566  33.727  29.658  1.00 77.30
ATOM    982  CB  GLN   132      56.536  32.293  30.218  1.00 77.68
ATOM    983  CG  GLN   132      55.424  31.387  29.676  1.00 78.41
ATOM    984  CD  GLN   132      55.823  30.611  28.436  1.00 78.88
ATOM    985  OE1 GLN   132      56.016  31.179  27.356  1.00 78.50
ATOM    986  NE2 GLN   132      55.951  29.294  28.587  1.00 79.41
ATOM    987  C   GLN   132      56.673  33.682  28.134  1.00 77.86
ATOM    988  O   GLN   132      57.769  33.638  27.574  1.00 77.91
ATOM    989  N   MSE   133      55.520  33.703  27.472  1.00 78.39
ATOM    990  CA  MSE   133      55.450  33.662  26.017  1.00 78.88
ATOM    991  CB  MSE   133      53.989  33.684  25.551  1.00 80.96
ATOM    992  CG  MSE   133      53.278  32.347  25.586  1.00 83.34
ATOM    993  SE  MSE   133      51.991  32.273  26.846  1.00 87.09
ATOM    994  CE  MSE   133      52.168  30.521  27.421  1.00 84.33
ATOM    995  C   MSE   133      56.174  34.812  25.333  1.00 77.90
ATOM    996  O   MSE   133      55.552  35.548  24.567  1.00 78.34
ATOM    997  N   LYS   134      57.470  34.973  25.587  1.00 75.97
ATOM    998  CA  LYS   134      58.225  36.053  24.949  1.00 73.96
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Figure 4

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ATOM    999  CB  LYS   134      58.976  36.879  25.997  1.00 73.14
ATOM   1000  CG  LYS   134      59.676  38.125  25.454  1.00 72.28
ATOM   1001  CD  LYS   134      58.697  39.250  25.141  1.00 70.99
ATOM   1002  CE  LYS   134      59.415  40.586  24.935  1.00 70.06
ATOM   1003  NZ  LYS   134      60.234  40.640  23.687  1.00 69.46
ATOM   1004  C   LYS   134      59.211  35.443  23.964  1.00 72.94
ATOM   1005  O   LYS   134      59.727  36.123  23.077  1.00 72.63
ATOM   1006  N   HIS   135      59.457  34.148  24.132  1.00 72.28
ATOM   1007  CA  HIS   135      60.377  33.411  23.275  1.00 71.52
ATOM   1008  CB  HIS   135      61.359  32.584  24.119  1.00 71.15
ATOM   1009  CG  HIS   135      60.719  31.448  24.859  1.00 70.88
ATOM   1010  CD2 HIS   135      60.908  30.109  24.773  1.00 70.87
ATOM   1011  ND1 HIS   135      59.750  31.635  25.822  1.00 70.81
ATOM   1012  CE1 HIS   135      59.370  30.462  26.298  1.00 70.56
ATOM   1013  NE2 HIS   135      60.057  29.519  25.678  1.00 70.85
ATOM   1014  C   HIS   135      59.584  32.482  22.365  1.00 71.26
ATOM   1015  O   HIS   135      60.152  31.818  21.499  1.00 71.53
ATOM   1016  N   LYS   136      58.272  32.434  22.574  1.00 70.85
ATOM   1017  CA  LYS   136      57.393  31.590  21.766  1.00 70.33
ATOM   1018  CB  LYS   136      56.077  31.329  22.508  1.00 69.64
ATOM   1019  CG  LYS   136      56.225  30.694  23.886  1.00 68.45
ATOM   1020  CD  LYS   136      56.740  29.271  23.783  1.00 68.01
ATOM   1021  CE  LYS   136      56.698  28.560  25.128  1.00 67.56
ATOM   1022  NZ  LYS   136      55.303  28.356  25.623  1.00 66.87
ATOM   1023  C   LYS   136      57.088  32.296  20.443  1.00 70.46
ATOM   1024  O   LYS   136      57.100  33.530  20.371  1.00 70.94
ATOM   1025  N   LYS   137      56.828  31.519  19.396  1.00 70.16
ATOM   1026  CA  LYS   137      56.505  32.096  18.096  1.00 69.80
ATOM   1027  CB  LYS   137      57.505  31.642  17.023  1.00 71.09
ATOM   1028  CG  LYS   137      57.602  30.132  16.801  1.00 71.73
ATOM   1029  CD  LYS   137      58.567  29.840  15.654  1.00 72.44
ATOM   1030  CE  LYS   137      58.915  28.363  15.545  1.00 72.39
ATOM   1031  NZ  LYS   137      59.919  28.136  14.463  1.00 72.59
ATOM   1032  C   LYS   137      55.097  31.685  17.702  1.00 68.73
ATOM   1033  O   LYS   137      54.799  31.476  16.524  1.00 69.92
ATOM   1034  N   LEU   138      54.243  31.579  18.716  1.00 66.57
ATOM   1035  CA  LEU   138      52.841  31.193  18.586  1.00 63.82
ATOM   1036  CB  LEU   138      52.057  31.788  19.748  1.00 63.11
ATOM   1037  CG  LEU   138      52.364  31.145  21.092  1.00 62.89
ATOM   1038  CD1 LEU   138      51.924  32.068  22.220  1.00 62.68
ATOM   1039  CD2 LEU   138      51.669  29.786  21.150  1.00 61.80
ATOM   1040  C   LEU   138      52.114  31.553  17.294  1.00 62.26
ATOM   1041  O   LEU   138      52.416  32.566  16.647  1.00 62.54
ATOM   1042  N   PRO   139      51.149  30.708  16.894  1.00 60.11
ATOM   1043  CD  PRO   139      50.841  29.394  17.489  1.00 59.82
ATOM   1044  CA  PRO   139      50.356  30.937  15.682  1.00 57.91
ATOM   1045  CB  PRO   139      49.761  29.564  15.398  1.00 58.05
ATOM   1046  CG  PRO   139      49.573  28.999  16.772  1.00 59.12
ATOM   1047  C   PRO   139      49.302  31.968  16.101  1.00 55.89
ATOM   1048  O   PRO   139      48.469  31.693  16.973  1.00 55.71
ATOM   1049  N   LEU   140      49.358  33.154  15.501  1.00 53.40
ATOM   1050  CA  LEU   140      48.440  34.237  15.850  1.00 50.78
ATOM   1051  CB  LEU   140      49.195  35.576  15.834  1.00 49.87
ATOM   1052  CG  LEU   140      48.452  36.893  16.091  1.00 49.01
ATOM   1053  CD1 LEU   140      49.414  37.933  16.646  1.00 48.17
ATOM   1054  CD2 LEU   140      47.825  37.389  14.801  1.00 48.88
ATOM   1055  C   LEU   140      47.169  34.359  15.018  1.00 49.13
ATOM   1056  O   LEU   140      47.211  34.368  13.785  1.00 49.12
ATOM   1057  N   GLY   141      46.040  34.441  15.722  1.00 46.93
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Figure 4

	ATOM	1058	CA	GLY	141	44.743	34.613	15.086	1.00	43.70
	ATOM	1059	C	GLY	141	44.324	36.041	15.402	1.00	41.11
	ATOM	1060	O	GLY	141	44.277	36.414	16.569	1.00	41.46
	ATOM	1061	N	PHE	142	44.018	36.842	14.388	1.00	38.27
5	ATOM	1062	CA	PHE	142	43.659	38.232	14.629	1.00	36.42
	ATOM	1063	CB	PHE	142	44.648	39.118	13.882	1.00	34.58
	ATOM	1064	CG	PHE	142	44.403	40.593	14.037	1.00	33.28
	ATOM	1065	CD1	PHE	142	43.941	41.124	15.229	1.00	32.86
	ATOM	1066	CD2	PHE	142	44.702	41.465	12.992	1.00	32.75
10	ATOM	1067	CE1	PHE	142	43.784	42.505	15.375	1.00	32.95
	ATOM	1068	CE2	PHE	142	44.551	42.845	13.125	1.00	31.57
	ATOM	1069	CZ	PHE	142	44.094	43.365	14.313	1.00	32.24
	ATOM	1070	C	PHE	142	42.224	38.652	14.300	1.00	36.83
	ATOM	1071	O	PHE	142	41.843	38.801	13.124	1.00	36.76
15	ATOM	1072	N	THR	143	41.423	38.848	15.347	1.00	35.96
	ATOM	1073	CA	THR	143	40.047	39.288	15.156	1.00	34.35
	ATOM	1074	CB	THR	143	39.179	38.997	16.373	1.00	33.98
	ATOM	1075	OG1	THR	143	38.947	37.586	16.472	1.00	33.45
	ATOM	1076	CG2	THR	143	37.854	39.750	16.255	1.00	33.35
20	ATOM	1077	C	THR	143	40.081	40.793	14.964	1.00	33.92
	ATOM	1078	O	THR	143	40.190	41.544	15.928	1.00	34.30
	ATOM	1079	N	PHE	144	40.009	41.227	13.716	1.00	33.00
	ATOM	1080	CA	PHE	144	40.029	42.649	13.383	1.00	31.69
	ATOM	1081	CB	PHE	144	40.891	42.842	12.132	1.00	29.18
25	ATOM	1082	CG	PHE	144	41.189	44.264	11.807	1.00	26.95
	ATOM	1083	CD1	PHE	144	41.727	45.108	12.763	1.00	26.21
	ATOM	1084	CD2	PHE	144	40.956	44.755	10.533	1.00	25.39
	ATOM	1085	CE1	PHE	144	42.026	46.428	12.450	1.00	26.79
	ATOM	1086	CE2	PHE	144	41.250	46.070	10.212	1.00	25.46
30	ATOM	1087	CZ	PHE	144	41.785	46.910	11.167	1.00	25.80
	ATOM	1088	C	PHE	144	38.562	42.981	13.112	1.00	32.02
	ATOM	1089	O	PHE	144	37.929	42.280	12.333	1.00	33.96
	ATOM	1090	N	SER	145	38.025	44.027	13.744	1.00	32.29
	ATOM	1091	CA	SER	145	36.602	44.387	13.600	1.00	31.56
35	ATOM	1092	CB	SER	145	35.993	44.689	14.968	1.00	31.79
	ATOM	1093	OG	SER	145	35.997	43.539	15.790	1.00	33.15
	ATOM	1094	C	SER	145	36.271	45.546	12.679	1.00	30.95
	ATOM	1095	O	SER	145	35.601	46.508	13.082	1.00	30.63
	ATOM	1096	N	PHE	146	36.723	45.456	11.439	1.00	30.27
40	ATOM	1097	CA	PHE	146	36.452	46.513	10.489	1.00	29.49
	ATOM	1098	CB	PHE	146	37.573	47.541	10.535	1.00	29.01
	ATOM	1099	CG	PHE	146	37.848	48.054	11.908	1.00	27.96
	ATOM	1100	CD1	PHE	146	38.654	47.336	12.775	1.00	28.87
	ATOM	1101	CD2	PHE	146	37.245	49.221	12.359	1.00	27.88
45	ATOM	1102	CE1	PHE	146	38.852	47.777	14.078	1.00	29.72
	ATOM	1103	CE2	PHE	146	37.434	49.670	13.659	1.00	26.92
	ATOM	1104	CZ	PHE	146	38.232	48.955	14.520	1.00	28.49
	ATOM	1105	C	PHE	146	36.318	45.937	9.093	1.00	29.49
	ATOM	1106	O	PHE	146	36.668	44.778	8.846	1.00	29.56
50	ATOM	1107	N	PRO	147	35.805	46.738	8.152	1.00	29.02
	ATOM	1108	CD	PRO	147	35.452	48.167	8.211	1.00	28.09
	ATOM	1109	CA	PRO	147	35.662	46.212	6.798	1.00	30.12
	ATOM	1110	CB	PRO	147	34.852	47.309	6.099	1.00	28.65
	ATOM	1111	CG	PRO	147	35.377	48.540	6.749	1.00	28.13
55	ATOM	1112	C	PRO	147	37.047	45.969	6.179	1.00	30.89
	ATOM	1113	O	PRO	147	37.938	46.821	6.263	1.00	32.17
	ATOM	1114	N	VAL	148	37.221	44.807	5.557	1.00	31.62
	ATOM	1115	CA	VAL	148	38.499	44.453	4.957	1.00	32.00
	ATOM	1116	CB	VAL	148	39.399	43.733	6.002	1.00	32.44

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ATOM   1117  CG1 VAL   148      40.471  42.940   5.311  1.00 33.36
ATOM   1118  CG2 VAL   148      40.035  44.758   6.934  1.00 32.04
ATOM   1119  C   VAL   148      38.351  43.557   3.733  1.00 31.54
ATOM   1120  O   VAL   148      37.937  42.402   3.858  1.00 30.91
ATOM   1121  N   ALA   149      38.688  44.091   2.560  1.00 31.66
ATOM   1122  CA  ALA   149      38.610  43.316   1.324  1.00 32.33
ATOM   1123  CB  ALA   149      38.834  44.213   0.120  1.00 31.16
ATOM   1124  C   ALA   149      39.723  42.288   1.428  1.00 33.43
ATOM   1125  O   ALA   149      40.882  42.653   1.431  1.00 35.59
ATOM   1126  N   HIS   150      39.387  41.008   1.535  1.00 33.73
ATOM   1127  CA  HIS   150      40.410  39.980   1.666  1.00 33.88
ATOM   1128  CB  HIS   150      39.868  38.780   2.450  1.00 34.82
ATOM   1129  CG  HIS   150      39.879  38.961   3.933  1.00 35.58
ATOM   1130  CD2 HIS   150      40.344  38.162   4.921  1.00 36.49
ATOM   1131  ND1 HIS   150      39.329  40.061   4.555  1.00 36.45
ATOM   1132  CE1 HIS   150      39.454  39.930   5.865  1.00 36.79
ATOM   1133  NE2 HIS   150      40.067  38.786   6.114  1.00 36.38
ATOM   1134  C   HIS   150      40.960  39.442   0.353  1.00 34.39
ATOM   1135  O   HIS   150      40.245  39.364  -0.655  1.00 34.56
ATOM   1136  N   ALA   151      42.239  39.068   0.380  1.00 34.73
ATOM   1137  CA  ALA   151      42.898  38.440  -0.762  1.00 34.53
ATOM   1138  CB  ALA   151      44.334  38.949  -0.919  1.00 34.86
ATOM   1139  C   ALA   151      42.894  36.968  -0.338  1.00 34.46
ATOM   1140  O   ALA   151      42.734  36.065  -1.161  1.00 34.16
ATOM   1141  N   ASP   152      43.050  36.754   0.970  1.00 34.36
ATOM   1142  CA  ASP   152      43.045  35.422   1.562  1.00 35.45
ATOM   1143  CB  ASP   152      44.335  34.687   1.214  1.00 37.69
ATOM   1144  CG  ASP   152      44.233  33.185   1.431  1.00 40.20
ATOM   1145  OD1 ASP   152      43.219  32.717   2.007  1.00 40.73
ATOM   1146  OD2 ASP   152      45.177  32.464   1.018  1.00 42.29
ATOM   1147  C   ASP   152      42.901  35.549   3.088  1.00 35.53
ATOM   1148  O   ASP   152      43.048  36.642   3.642  1.00 35.08
ATOM   1149  N   ILE   153      42.627  34.433   3.762  1.00 35.49
ATOM   1150  CA  ILE   153      42.436  34.427   5.213  1.00 35.75
ATOM   1151  CB  ILE   153      42.258  32.984   5.754  1.00 35.32
ATOM   1152  CG2 ILE   153      43.609  32.316   5.937  1.00 34.16
ATOM   1153  CG1 ILE   153      41.593  33.022   7.130  1.00 35.44
ATOM   1154  CD1 ILE   153      40.225  33.697   7.131  1.00 36.43
ATOM   1155  C   ILE   153      43.571  35.079   6.011  1.00 36.77
ATOM   1156  O   ILE   153      43.450  35.278   7.229  1.00 36.40
ATOM   1157  N   ASP   154      44.665  35.411   5.332  1.00 37.10
ATOM   1158  CA  ASP   154      45.815  36.003   6.000  1.00 37.27
ATOM   1159  CB  ASP   154      46.982  35.013   5.991  1.00 38.98
ATOM   1160  CG  ASP   154      47.795  35.079   4.703  1.00 41.58
ATOM   1161  OD1 ASP   154      47.215  34.890   3.605  1.00 42.46
ATOM   1162  OD2 ASP   154      49.022  35.331   4.789  1.00 42.65
ATOM   1163  C   ASP   154      46.233  37.287   5.307  1.00 36.74
ATOM   1164  O   ASP   154      47.360  37.751   5.471  1.00 37.07
ATOM   1165  N   ALA   155      45.328  37.865   4.531  1.00 35.91
ATOM   1166  CA  ALA   155      45.650  39.093   3.830  1.00 36.20
ATOM   1167  CB  ALA   155      46.522  38.771   2.621  1.00 36.22
ATOM   1168  C   ALA   155      44.412  39.864   3.387  1.00 36.20
ATOM   1169  O   ALA   155      43.490  39.289   2.820  1.00 36.87
ATOM   1170  N   GLY   156      44.402  41.168   3.642  1.00 36.26
ATOM   1171  CA  GLY   156      43.279  41.997   3.245  1.00 37.08
ATOM   1172  C   GLY   156      43.481  43.446   3.647  1.00 38.10
ATOM   1173  O   GLY   156      44.027  43.727   4.711  1.00 38.52
ATOM   1174  N   ILE   157      43.052  44.377   2.805  1.00 39.16
ATOM   1175  CA  ILE   157      43.203  45.789   3.125  1.00 41.42
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ATOM   1176  CB  ILE   157      43.389  46.646   1.842  1.00 42.84
ATOM   1177  CG2 ILE   157      44.844  46.550   1.349  1.00 44.32
ATOM   1178  CG1 ILE   157      42.399  46.193   0.761  1.00 43.93
ATOM   1179  CD1 ILE   157      42.630  46.838  -0.615  1.00 44.55
ATOM   1180  C   ILE   157      42.010  46.331   3.921  1.00 42.26
ATOM   1181  O   ILE   157      40.864  45.912   3.732  1.00 42.28
ATOM   1182  N   LEU   158      42.300  47.259   4.824  1.00 42.54
ATOM   1183  CA  LEU   158      41.283  47.873   5.648  1.00 43.22
ATOM   1184  CB  LEU   158      41.928  48.504   6.884  1.00 44.12
ATOM   1185  CG  LEU   158      41.090  49.514   7.670  1.00 44.84
ATOM   1186  CD1 LEU   158      40.020  48.782   8.472  1.00 45.23
ATOM   1187  CD2 LEU   158      42.006  50.320   8.590  1.00 45.09
ATOM   1188  C   LEU   158      40.548  48.947   4.855  1.00 43.56
ATOM   1189  O   LEU   158      40.984  50.099   4.801  1.00 43.77
ATOM   1190  N   LEU   159      39.434  48.569   4.239  1.00 43.40
ATOM   1191  CA  LEU   159      38.634  49.508   3.465  1.00 43.01
ATOM   1192  CB  LEU   159      37.238  48.935   3.280  1.00 43.36
ATOM   1193  CG  LEU   159      37.279  47.599   2.539  1.00 43.44
ATOM   1194  CD1 LEU   159      36.020  46.808   2.829  1.00 44.00
ATOM   1195  CD2 LEU   159      37.443  47.857   1.050  1.00 42.93
ATOM   1196  C   LEU   159      38.564  50.879   4.139  1.00 42.62
ATOM   1197  O   LEU   159      38.745  51.905   3.488  1.00 43.03
ATOM   1198  N   ASN   160      38.297  50.902   5.440  1.00 42.20
ATOM   1199  CA  ASN   160      38.243  52.169   6.170  1.00 41.99
ATOM   1200  CB  ASN   160      37.347  53.197   5.447  1.00 42.23
ATOM   1201  CG  ASN   160      35.913  52.733   5.295  1.00 43.38
ATOM   1202  OD1 ASN   160      35.225  53.102   4.334  1.00 42.38
ATOM   1203  ND2 ASN   160      35.444  51.934   6.250  1.00 44.48
ATOM   1204  C   ASN   160      37.813  51.988   7.616  1.00 41.13
ATOM   1205  O   ASN   160      37.359  50.913   8.011  1.00 41.17
ATOM   1206  N   TRP   161      37.980  53.043   8.403  1.00 40.24
ATOM   1207  CA  TRP   161      37.652  53.004   9.824  1.00 39.69
ATOM   1208  CB  TRP   161      38.522  54.003  10.602  1.00 39.33
ATOM   1209  CG  TRP   161      39.987  53.640  10.769  1.00 39.07
ATOM   1210  CD2 TRP   161      40.527  52.469  11.411  1.00 38.63
ATOM   1211  CE2 TRP   161      41.931  52.616  11.438  1.00 38.27
ATOM   1212  CE3 TRP   161      39.960  51.317  11.972  1.00 38.43
ATOM   1213  CD1 TRP   161      41.060  54.417  10.436  1.00 38.40
ATOM   1214  NE1 TRP   161      42.228  53.812  10.840  1.00 38.42
ATOM   1215  CZ2 TRP   161      42.778  51.659  12.000  1.00 38.26
ATOM   1216  CZ3 TRP   161      40.809  50.357  12.538  1.00 38.07
ATOM   1217  CH2 TRP   161      42.200  50.540  12.545  1.00 38.37
ATOM   1218  C   TRP   161      36.196  53.301  10.150  1.00 39.07
ATOM   1219  O   TRP   161      35.578  54.193   9.562  1.00 39.38
ATOM   1220  N   THR   162      35.668  52.555  11.114  1.00 38.45
ATOM   1221  CA  THR   162      34.302  52.734  11.593  1.00 38.37
ATOM   1222  CB  THR   162      33.381  51.600  11.125  1.00 37.71
ATOM   1223  OG1 THR   162      33.926  50.338  11.548  1.00 37.02
ATOM   1224  CG2 THR   162      33.226  51.635   9.617  1.00 36.52
ATOM   1225  C   THR   162      34.357  52.702  13.121  1.00 38.24
ATOM   1226  O   THR   162      35.405  52.443  13.703  1.00 37.86
ATOM   1227  N   LYS   163      33.231  52.968  13.770  1.00 38.99
ATOM   1228  CA  LYS   163      33.192  52.941  15.222  1.00 39.72
ATOM   1229  CB  LYS   163      33.510  51.528  15.728  1.00 38.16
ATOM   1230  CG  LYS   163      32.467  50.487  15.311  1.00 36.62
ATOM   1231  CD  LYS   163      32.727  49.108  15.918  1.00 34.66
ATOM   1232  CE  LYS   163      33.829  48.349  15.195  1.00 33.22
ATOM   1233  NZ  LYS   163      34.068  47.031  15.850  1.00 32.19
ATOM   1234  C   LYS   163      34.142  53.956  15.848  1.00 40.71
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ATOM   1235  O   LYS  163      34.690  53.723  16.931  1.00 40.69
ATOM   1236  N   GLY  164      34.338  55.076  15.156  1.00 41.81
ATOM   1237  CA  GLY  164      35.187  56.139  15.672  1.00 43.90
ATOM   1238  C   GLY  164      36.685  56.031  15.463  1.00 45.41
ATOM   1239  O   GLY  164      37.375  57.055  15.381  1.00 45.25
ATOM   1240  N   PHE  165      37.190  54.802  15.397  1.00 47.06
ATOM   1241  CA  PHE  165      38.613  54.560  15.197  1.00 48.70
ATOM   1242  CB  PHE  165      38.852  53.117  14.767  1.00 47.20
ATOM   1243  CG  PHE  165      39.290  52.222  15.870  1.00 45.64
ATOM   1244  CD1 PHE  165      38.443  51.937  16.929  1.00 45.87
ATOM   1245  CD2 PHE  165      40.544  51.632  15.833  1.00 45.19
ATOM   1246  CE1 PHE  165      38.840  51.064  17.945  1.00 46.28
ATOM   1247  CE2 PHE  165      40.952  50.763  16.834  1.00 45.80
ATOM   1248  CZ  PHE  165      40.098  50.475  17.896  1.00 45.96
ATOM   1249  C   PHE  165      39.250  55.471  14.154  1.00 50.94
ATOM   1250  O   PHE  165      38.633  55.823  13.143  1.00 50.36
ATOM   1251  N   LYS  166      40.500  55.838  14.415  1.00 53.77
ATOM   1252  CA  LYS  166      41.275  56.680  13.514  1.00 56.56
ATOM   1253  CB  LYS  166      41.050  58.170  13.822  1.00 56.16
ATOM   1254  CG  LYS  166      39.720  58.697  13.290  1.00 56.44
ATOM   1255  CD  LYS  166      39.524  58.320  11.812  1.00 56.54
ATOM   1256  CE  LYS  166      38.131  58.694  11.305  1.00 56.74
ATOM   1257  NZ  LYS  166      37.863  58.198   9.922  1.00 56.86
ATOM   1258  C   LYS  166      42.751  56.322  13.640  1.00 58.33
ATOM   1259  O   LYS  166      43.180  55.747  14.651  1.00 58.69
ATOM   1260  N   ALA  167      43.510  56.647  12.597  1.00 59.76
ATOM   1261  CA  ALA  167      44.943  56.375  12.543  1.00 61.43
ATOM   1262  CB  ALA  167      45.220  54.901  12.834  1.00 60.92
ATOM   1263  C   ALA  167      45.401  56.725  11.137  1.00 62.76
ATOM   1264  O   ALA  167      45.147  55.967  10.197  1.00 63.38
ATOM   1265  N   SER  168      46.066  57.872  10.999  1.00 63.98
ATOM   1266  CA  SER  168      46.556  58.345   9.704  1.00 64.43
ATOM   1267  CB  SER  168      47.636  59.414   9.903  1.00 64.96
ATOM   1268  OG  SER  168      47.130  60.546  10.594  1.00 65.76
ATOM   1269  C   SER  168      47.115  57.216   8.846  1.00 64.59
ATOM   1270  O   SER  168      47.805  56.322   9.347  1.00 64.35
ATOM   1271  N   GLY  169      46.800  57.260   7.553  1.00 64.75
ATOM   1272  CA  GLY  169      47.280  56.245   6.632  1.00 65.55
ATOM   1273  C   GLY  169      47.158  54.821   7.142  1.00 65.88
ATOM   1274  O   GLY  169      48.151  54.097   7.255  1.00 65.72
ATOM   1275  N   ALA  170      45.936  54.416   7.465  1.00 66.32
ATOM   1276  CA  ALA  170      45.699  53.065   7.947  1.00 66.82
ATOM   1277  CB  ALA  170      44.930  53.100   9.256  1.00 66.65
ATOM   1278  C   ALA  170      44.890  52.346   6.879  1.00 67.02
ATOM   1279  O   ALA  170      45.209  51.226   6.477  1.00 67.31
ATOM   1280  N   GLU  171      43.847  53.017   6.410  1.00 66.85
ATOM   1281  CA  GLU  171      42.979  52.463   5.387  1.00 66.80
ATOM   1282  CB  GLU  171      41.705  53.292   5.287  1.00 67.90
ATOM   1283  CG  GLU  171      41.958  54.783   5.279  1.00 69.27
ATOM   1284  CD  GLU  171      40.850  55.552   4.590  1.00 70.17
ATOM   1285  OE1 GLU  171      40.789  55.506   3.340  1.00 70.45
ATOM   1286  OE2 GLU  171      40.038  56.191   5.296  1.00 70.67
ATOM   1287  C   GLU  171      43.666  52.427   4.032  1.00 65.92
ATOM   1288  O   GLU  171      44.469  53.301   3.711  1.00 66.22
ATOM   1289  N   GLY  172      43.339  51.408   3.242  1.00 64.69
ATOM   1290  CA  GLY  172      43.922  51.265   1.925  1.00 62.79
ATOM   1291  C   GLY  172      45.096  50.312   1.882  1.00 61.61
ATOM   1292  O   GLY  172      45.493  49.884   0.805  1.00 61.59
ATOM   1293  N   ASN  173      45.643  49.965   3.045  1.00 60.93
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Figure 4

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ATOM   1294  CA  ASN  173      46.800  49.065   3.115  1.00 60.42
ATOM   1295  CB  ASN  173      47.922  49.722   3.913  1.00 61.72
ATOM   1296  CG  ASN  173      48.035  51.201   3.631  1.00 62.78
ATOM   1297  OD1 ASN  173      48.367  51.605   2.515  1.00 63.29
ATOM   1298  ND2 ASN  173      47.741  52.024   4.637  1.00 63.06
ATOM   1299  C   ASN  173      46.463  47.747   3.771  1.00 59.26
ATOM   1300  O   ASN  173      45.440  47.624   4.430  1.00 59.57
ATOM   1301  N   ASN  174      47.336  46.763   3.598  1.00 58.79
ATOM   1302  CA  ASN  174      47.126  45.447   4.196  1.00 58.46
ATOM   1303  CB  ASN  174      48.264  44.495   3.793  1.00 57.45
ATOM   1304  CG  ASN  174      48.104  43.093   4.375  1.00 57.22
ATOM   1305  OD1 ASN  174      48.757  42.144   3.924  1.00 56.21
ATOM   1306  ND2 ASN  174      47.245  42.957   5.382  1.00 56.76
ATOM   1307  C   ASN  174      47.083  45.615   5.712  1.00 58.42
ATOM   1308  O   ASN  174      47.927  46.302   6.281  1.00 59.03
ATOM   1309  N   VAL  175      46.091  45.008   6.359  1.00 58.23
ATOM   1310  CA  VAL  175      45.966  45.106   7.809  1.00 57.79
ATOM   1311  CB  VAL  175      44.544  44.765   8.295  1.00 57.69
ATOM   1312  CG1 VAL  175      44.461  44.933   9.807  1.00 56.81
ATOM   1313  CG2 VAL  175      43.531  45.665   7.603  1.00 57.69
ATOM   1314  C   VAL  175      46.944  44.150   8.470  1.00 57.62
ATOM   1315  O   VAL  175      47.734  44.560   9.319  1.00 57.89
ATOM   1316  N   VAL  176      46.896  42.878   8.086  1.00 57.24
ATOM   1317  CA  VAL  176      47.818  41.904   8.660  1.00 57.25
ATOM   1318  CB  VAL  176      47.638  40.501   8.037  1.00 57.27
ATOM   1319  CG1 VAL  176      48.597  39.511   8.701  1.00 56.21
ATOM   1320  CG2 VAL  176      46.196  40.035   8.199  1.00 56.28
ATOM   1321  C   VAL  176      49.232  42.396   8.362  1.00 57.38
ATOM   1322  O   VAL  176      50.212  41.911   8.926  1.00 57.30
ATOM   1323  N   GLY  177      49.319  43.374   7.467  1.00 57.41
ATOM   1324  CA  GLY  177      50.605  43.939   7.103  1.00 57.60
ATOM   1325  C   GLY  177      51.135  44.878   8.170  1.00 57.50
ATOM   1326  O   GLY  177      52.171  44.605   8.781  1.00 58.09
ATOM   1327  N   LEU  178      50.425  45.982   8.396  1.00 56.68
ATOM   1328  CA  LEU  178      50.837  46.959   9.396  1.00 55.42
ATOM   1329  CB  LEU  178      49.710  47.968   9.646  1.00 55.02
ATOM   1330  CG  LEU  178      49.394  48.906   8.466  1.00 54.15
ATOM   1331  CD1 LEU  178      48.158  49.743   8.766  1.00 53.80
ATOM   1332  CD2 LEU  178      50.588  49.815   8.197  1.00 54.17
ATOM   1333  C   LEU  178      51.247  46.279  10.701  1.00 54.84
ATOM   1334  O   LEU  178      52.177  46.717  11.375  1.00 55.07
ATOM   1335  N   LEU  179      50.575  45.192  11.050  1.00 53.85
ATOM   1336  CA  LEU  179      50.917  44.491  12.274  1.00 53.57
ATOM   1337  CB  LEU  179      49.882  43.409  12.582  1.00 52.75
ATOM   1338  CG  LEU  179      50.099  42.671  13.907  1.00 52.23
ATOM   1339  CD1 LEU  179      49.689  43.580  15.056  1.00 51.63
ATOM   1340  CD2 LEU  179      49.286  41.381  13.935  1.00 51.34
ATOM   1341  C   LEU  179      52.286  43.845  12.128  1.00 54.26
ATOM   1342  O   LEU  179      53.070  43.796  13.075  1.00 54.60
ATOM   1343  N   ARG  180      52.576  43.343  10.932  1.00 54.59
ATOM   1344  CA  ARG  180      53.855  42.679  10.688  1.00 54.08
ATOM   1345  CB  ARG  180      53.824  41.911   9.357  1.00 52.59
ATOM   1346  CG  ARG  180      53.273  40.498   9.515  1.00 50.37
ATOM   1347  CD  ARG  180      53.276  39.702   8.223  1.00 47.24
ATOM   1348  NE  ARG  180      52.610  38.420   8.425  1.00 45.06
ATOM   1349  CZ  ARG  180      51.979  37.754   7.462  1.00 43.97
ATOM   1350  NH1 ARG  180      51.935  38.256   6.226  1.00 42.53
ATOM   1351  NH2 ARG  180      51.366  36.601   7.735  1.00 42.95
ATOM   1352  C   ARG  180      55.059  43.605  10.732  1.00 54.76
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Figure 4

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ATOM   1353  O   ARG   180      56.009  43.343  11.473  1.00 54.65
ATOM   1354  N   ASP   181      55.036  44.681   9.951  1.00 55.34
ATOM   1355  CA  ASP   181      56.169  45.593   9.972  1.00 56.60
ATOM   1356  CB  ASP   181      56.266  46.386   8.649  1.00 56.43
ATOM   1357  CG  ASP   181      55.132  47.382   8.448  1.00 55.64
ATOM   1358  OD1 ASP   181      54.658  47.483   7.294  1.00 55.20
ATOM   1359  OD2 ASP   181      54.734  48.076   9.416  1.00 55.23
ATOM   1360  C   ASP   181      56.115  46.514  11.199  1.00 57.64
ATOM   1361  O   ASP   181      56.510  47.685  11.153  1.00 57.96
ATOM   1362  N   ALA   182      55.634  45.947  12.303  1.00 57.87
ATOM   1363  CA  ALA   182      55.524  46.646  13.577  1.00 57.84
ATOM   1364  CB  ALA   182      54.078  47.048  13.836  1.00 58.19
ATOM   1365  C   ALA   182      56.013  45.683  14.657  1.00 57.83
ATOM   1366  O   ALA   182      56.681  46.094  15.611  1.00 58.32
ATOM   1367  N   ILE   183      55.669  44.404  14.505  1.00 57.85
ATOM   1368  CA  ILE   183      56.109  43.381  15.448  1.00 57.40
ATOM   1369  CB  ILE   183      55.374  42.036  15.233  1.00 56.09
ATOM   1370  CG2 ILE   183      56.025  40.932  16.074  1.00 55.25
ATOM   1371  CG1 ILE   183      53.904  42.174  15.628  1.00 55.30
ATOM   1372  CD1 ILE   183      53.115  40.881  15.505  1.00 54.14
ATOM   1373  C   ILE   183      57.600  43.164  15.199  1.00 58.51
ATOM   1374  O   ILE   183      58.294  42.531  16.002  1.00 59.24
ATOM   1375  N   LYS   184      58.093  43.689  14.077  1.00 59.04
ATOM   1376  CA  LYS   184      59.508  43.550  13.757  1.00 59.19
ATOM   1377  CB  LYS   184      59.719  43.243  12.268  1.00 59.15
ATOM   1378  CG  LYS   184      59.356  44.354  11.310  1.00 58.36
ATOM   1379  CD  LYS   184      59.566  43.897   9.868  1.00 58.59
ATOM   1380  CE  LYS   184      58.637  42.735   9.500  1.00 59.26
ATOM   1381  NZ  LYS   184      58.751  42.306   8.067  1.00 59.63
ATOM   1382  C   LYS   184      60.270  44.806  14.155  1.00 59.27
ATOM   1383  O   LYS   184      61.382  44.705  14.667  1.00 59.28
ATOM   1384  N   ARG   185      59.695  45.984  13.923  1.00 59.21
ATOM   1385  CA  ARG   185      60.383  47.211  14.331  1.00 59.69
ATOM   1386  CB  ARG   185      59.545  48.458  14.060  1.00 59.70
ATOM   1387  CG  ARG   185      59.278  48.772  12.610  1.00 60.85
ATOM   1388  CD  ARG   185      59.138  50.280  12.443  1.00 60.89
ATOM   1389  NE  ARG   185      58.121  50.628  11.459  1.00 62.26
ATOM   1390  CZ  ARG   185      56.819  50.403  11.620  1.00 61.84
ATOM   1391  NH1 ARG   185      56.372  49.828  12.731  1.00 61.22
ATOM   1392  NH2 ARG   185      55.966  50.754  10.666  1.00 62.23
ATOM   1393  C   ARG   185      60.574  47.104  15.836  1.00 60.41
ATOM   1394  O   ARG   185      61.630  47.430  16.384  1.00 60.45
ATOM   1395  N   ARG   186      59.518  46.633  16.489  1.00 61.07
ATOM   1396  CA  ARG   186      59.489  46.460  17.933  1.00 61.42
ATOM   1397  CB  ARG   186      58.066  46.055  18.358  1.00 61.16
ATOM   1398  CG  ARG   186      57.666  46.433  19.786  1.00 61.08
ATOM   1399  CD  ARG   186      58.249  45.473  20.828  1.00 60.87
ATOM   1400  NE  ARG   186      57.917  45.894  22.188  1.00 61.44
ATOM   1401  CZ  ARG   186      58.294  45.246  23.288  1.00 60.67
ATOM   1402  NH1 ARG   186      59.024  44.133  23.201  1.00 60.28
ATOM   1403  NH2 ARG   186      57.942  45.712  24.481  1.00 61.46
ATOM   1404  C   ARG   186      60.516  45.399  18.344  1.00 61.85
ATOM   1405  O   ARG   186      60.980  44.610  17.514  1.00 62.16
ATOM   1406  N   GLY   187      60.873  45.401  19.628  1.00 62.07
ATOM   1407  CA  GLY   187      61.843  44.455  20.157  1.00 62.22
ATOM   1408  C   GLY   187      61.591  43.017  19.754  1.00 62.50
ATOM   1409  O   GLY   187      60.541  42.692  19.202  1.00 62.37
ATOM   1410  N   ASP   188      62.556  42.148  20.036  1.00 63.08
ATOM   1411  CA  ASP   188      62.414  40.746  19.684  1.00 62.67
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ATOM   1412  CB  ASP   188      63.465  39.873  20.373  1.00 61.80
ATOM   1413  CG  ASP   188      63.027  38.409  20.468  1.00 60.64
ATOM   1414  OD1 ASP   188      62.125  38.107  21.289  1.00 60.77
ATOM   1415  OD2 ASP   188      63.565  37.563  19.715  1.00 60.43
ATOM   1416  C   ASP   188      61.047  40.193  20.022  1.00 63.58
ATOM   1417  O   ASP   188      60.441  40.539  21.044  1.00 62.69
ATOM   1418  N   PHE   189      60.599  39.309  19.138  1.00 64.49
ATOM   1419  CA  PHE   189      59.327  38.632  19.249  1.00 64.75
ATOM   1420  CB  PHE   189      58.233  39.629  19.598  1.00 64.84
ATOM   1421  CG  PHE   189      56.886  39.010  19.689  1.00 65.46
ATOM   1422  CD1 PHE   189      56.707  37.824  20.402  1.00 65.54
ATOM   1423  CD2 PHE   189      55.795  39.592  19.052  1.00 65.28
ATOM   1424  CE1 PHE   189      55.455  37.224  20.481  1.00 65.61
ATOM   1425  CE2 PHE   189      54.542  39.007  19.122  1.00 65.71
ATOM   1426  CZ  PHE   189      54.369  37.819  19.839  1.00 65.67
ATOM   1427  C   PHE   189      59.018  37.952  17.919  1.00 65.33
ATOM   1428  O   PHE   189      58.921  38.609  16.881  1.00 64.91
ATOM   1429  N   GLU   190      58.879  36.631  17.956  1.00 66.13
ATOM   1430  CA  GLU   190      58.584  35.854  16.752  1.00 66.57
ATOM   1431  CB  GLU   190      59.387  34.545  16.755  1.00 66.34
ATOM   1432  CG  GLU   190      60.778  34.649  17.389  1.00 64.66
ATOM   1433  CD  GLU   190      61.908  34.356  16.411  1.00 64.02
ATOM   1434  OE1 GLU   190      63.054  34.161  16.874  1.00 63.09
ATOM   1435  OE2 GLU   190      61.658  34.327  15.186  1.00 63.04
ATOM   1436  C   GLU   190      57.093  35.528  16.745  1.00 67.09
ATOM   1437  O   GLU   190      56.609  34.828  17.638  1.00 67.36
ATOM   1438  N   MSE   191      56.367  36.030  15.747  1.00 67.05
ATOM   1439  CA  MSE   191      54.928  35.775  15.666  1.00 66.65
ATOM   1440  CB  MSE   191      54.164  36.920  16.347  1.00 69.47
ATOM   1441  CG  MSE   191      52.867  36.492  17.037  1.00 72.30
ATOM   1442  SE  MSE   191      53.120  35.293  18.409  1.00 78.56
ATOM   1443  CE  MSE   191      51.941  35.893  19.581  1.00 75.88
ATOM   1444  C   MSE   191      54.412  35.590  14.230  1.00 64.85
ATOM   1445  O   MSE   191      54.399  36.538  13.435  1.00 64.30
ATOM   1446  N   ASP   192      53.977  34.368  13.910  1.00 62.82
ATOM   1447  CA  ASP   192      53.449  34.051  12.580  1.00 60.76
ATOM   1448  CB  ASP   192      53.774  32.607  12.207  1.00 61.24
ATOM   1449  CG  ASP   192      55.210  32.427  11.792  1.00 61.76
ATOM   1450  OD1 ASP   192      55.684  33.219  10.947  1.00 62.45
ATOM   1451  OD2 ASP   192      55.863  31.492  12.299  1.00 62.32
ATOM   1452  C   ASP   192      51.942  34.266  12.459  1.00 59.03
ATOM   1453  O   ASP   192      51.143  33.375  12.767  1.00 58.37
ATOM   1454  N   VAL   193      51.567  35.453  11.991  1.00 57.00
ATOM   1455  CA  VAL   193      50.167  35.818  11.818  1.00 54.85
ATOM   1456  CB  VAL   193      50.034  37.305  11.454  1.00 55.09
ATOM   1457  CG1 VAL   193      48.568  37.712  11.448  1.00 54.84
ATOM   1458  CG2 VAL   193      50.826  38.146  12.441  1.00 54.87
ATOM   1459  C   VAL   193      49.473  34.977  10.746  1.00 53.19
ATOM   1460  O   VAL   193      49.500  35.303   9.555  1.00 52.03
ATOM   1461  N   VAL   194      48.854  33.894  11.205  1.00 51.82
ATOM   1462  CA  VAL   194      48.126  32.949  10.367  1.00 50.66
ATOM   1463  CB  VAL   194      47.841  31.644  11.174  1.00 51.08
ATOM   1464  CG1 VAL   194      46.686  30.860  10.554  1.00 52.09
ATOM   1465  CG2 VAL   194      49.091  30.778  11.211  1.00 51.33
ATOM   1466  C   VAL   194      46.798  33.498   9.808  1.00 49.99
ATOM   1467  O   VAL   194      46.677  33.726   8.602  1.00 49.40
ATOM   1468  N   ALA   195      45.813  33.723  10.683  1.00 48.93
ATOM   1469  CA  ALA   195      44.499  34.193  10.251  1.00 47.60
ATOM   1470  CB  ALA   195      43.467  33.123  10.572  1.00 47.58
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Figure 4

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ATOM   1471  C   ALA  195      43.992  35.546  10.760  1.00 46.68
ATOM   1472  O   ALA  195      44.344  35.996  11.851  1.00 46.16
ATOM   1473  N   MSE  196      43.157  36.182   9.940  1.00 45.43
ATOM   1474  CA  MSE  196      42.521  37.459  10.279  1.00 44.60
ATOM   1475  CB  MSE  196      43.079  38.623   9.451  1.00 45.32
ATOM   1476  CG  MSE  196      42.329  39.925   9.716  1.00 47.29
ATOM   1477  SE  MSE  196      42.937  41.426   8.852  1.00 53.21
ATOM   1478  CE  MSE  196      44.264  41.920   9.982  1.00 51.44
ATOM   1479  C   MSE  196      41.019  37.333  10.002  1.00 43.09
ATOM   1480  O   MSE  196      40.610  36.973   8.892  1.00 43.71
ATOM   1481  N   VAL  197      40.190  37.631  10.996  1.00 40.47
ATOM   1482  CA  VAL  197      38.751  37.514  10.799  1.00 37.00
ATOM   1483  CB  VAL  197      38.240  36.228  11.458  1.00 37.31
ATOM   1484  CG1 VAL  197      38.840  35.004  10.766  1.00 36.64
ATOM   1485  CG2 VAL  197      38.643  36.217  12.914  1.00 36.88
ATOM   1486  C   VAL  197      37.991  38.710  11.354  1.00 35.22
ATOM   1487  O   VAL  197      38.561  39.544  12.057  1.00 35.21
ATOM   1488  N   ASN  198      36.708  38.801  11.015  1.00 33.39
ATOM   1489  CA  ASN  198      35.830  39.883  11.491  1.00 30.23
ATOM   1490  CB  ASN  198      34.740  40.175  10.446  1.00 30.65
ATOM   1491  CG  ASN  198      33.801  41.309  10.852  1.00 31.35
ATOM   1492  OD1 ASN  198      32.907  41.128  11.686  1.00 32.70
ATOM   1493  ND2 ASN  198      33.997  42.486  10.251  1.00 30.53
ATOM   1494  C   ASN  198      35.217  39.356  12.780  1.00 28.41
ATOM   1495  O   ASN  198      35.052  38.143  12.937  1.00 26.14
ATOM   1496  N   ASP  199      34.892  40.252  13.711  1.00 27.77
ATOM   1497  CA  ASP  199      34.325  39.816  14.990  1.00 26.87
ATOM   1498  CB  ASP  199      34.156  41.007  15.945  1.00 26.75
ATOM   1499  CG  ASP  199      33.254  42.097  15.396  1.00 26.24
ATOM   1500  OD1 ASP  199      33.221  42.292  14.167  1.00 26.90
ATOM   1501  OD2 ASP  199      32.587  42.777  16.205  1.00 26.19
ATOM   1502  C   ASP  199      33.027  39.034  14.843  1.00 26.43
ATOM   1503  O   ASP  199      32.715  38.188  15.684  1.00 27.02
ATOM   1504  N   THR  200      32.291  39.292  13.763  1.00 25.45
ATOM   1505  CA  THR  200      31.050  38.585  13.510  1.00 25.65
ATOM   1506  CB  THR  200      30.261  39.193  12.339  1.00 25.75
ATOM   1507  OG1 THR  200      31.008  39.044  11.130  1.00 26.04
ATOM   1508  CG2 THR  200      30.002  40.672  12.573  1.00 26.48
ATOM   1509  C   THR  200      31.383  37.155  13.143  1.00 26.96
ATOM   1510  O   THR  200      30.832  36.211  13.712  1.00 27.62
ATOM   1511  N   VAL  201      32.295  36.990  12.189  1.00 28.07
ATOM   1512  CA  VAL  201      32.695  35.654  11.742  1.00 28.50
ATOM   1513  CB  VAL  201      33.785  35.726  10.665  1.00 29.26
ATOM   1514  CG1 VAL  201      34.056  34.332  10.123  1.00 31.22
ATOM   1515  CG2 VAL  201      33.370  36.684   9.546  1.00 27.90
ATOM   1516  C   VAL  201      33.231  34.818  12.901  1.00 29.16
ATOM   1517  O   VAL  201      32.816  33.676  13.101  1.00 29.44
ATOM   1518  N   ALA  202      34.156  35.395  13.663  1.00 30.31
ATOM   1519  CA  ALA  202      34.752  34.710  14.812  1.00 32.23
ATOM   1520  CB  ALA  202      35.591  35.705  15.643  1.00 31.72
ATOM   1521  C   ALA  202      33.688  34.070  15.696  1.00 33.37
ATOM   1522  O   ALA  202      33.789  32.894  16.073  1.00 34.14
ATOM   1523  N   THR  203      32.667  34.858  16.019  1.00 34.41
ATOM   1524  CA  THR  203      31.566  34.422  16.870  1.00 35.37
ATOM   1525  CB  THR  203      30.614  35.604  17.117  1.00 36.27
ATOM   1526  OG1 THR  203      31.370  36.708  17.645  1.00 37.04
ATOM   1527  CG2 THR  203      29.500  35.213  18.090  1.00 35.19
ATOM   1528  C   THR  203      30.800  33.260  16.242  1.00 36.08
ATOM   1529  O   THR  203      30.538  32.241  16.891  1.00 35.34
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Figure 4

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ATOM   1530  N   MSE   204      30.433  33.415  14.978  1.00 36.89
ATOM   1531  CA  MSE   204      29.722  32.348  14.299  1.00 37.94
ATOM   1532  CB  MSE   204      29.582  32.665  12.811  1.00 39.76
ATOM   1533  CG  MSE   204      29.065  31.504  11.954  1.00 40.74
ATOM   1534  SE  MSE   204      29.135  31.967  10.181  1.00 45.75
ATOM   1535  CE  MSE   204      30.643  31.057   9.627  1.00 45.26
ATOM   1536  C   MSE   204      30.531  31.075  14.465  1.00 38.36
ATOM   1537  O   MSE   204      30.024  30.064  14.954  1.00 37.86
ATOM   1538  N   ILE   205      31.798  31.148  14.061  1.00 38.79
ATOM   1539  CA  ILE   205      32.696  30.008  14.137  1.00 40.09
ATOM   1540  CB  ILE   205      34.178  30.451  13.981  1.00 39.81
ATOM   1541  CG2 ILE   205      35.098  29.240  14.072  1.00 39.47
ATOM   1542  CG1 ILE   205      34.398  31.112  12.616  1.00 39.46
ATOM   1543  CD1 ILE   205      34.250  30.158  11.425  1.00 39.34
ATOM   1544  C   ILE   205      32.527  29.215  15.440  1.00 41.34
ATOM   1545  O   ILE   205      32.121  28.050  15.408  1.00 41.41
ATOM   1546  N   SER   206      32.812  29.830  16.584  1.00 42.01
ATOM   1547  CA  SER   206      32.683  29.112  17.849  1.00 43.71
ATOM   1548  CB  SER   206      32.999  30.038  19.013  1.00 43.57
ATOM   1549  OG  SER   206      32.149  31.163  18.971  1.00 44.54
ATOM   1550  C   SER   206      31.306  28.494  18.056  1.00 44.83
ATOM   1551  O   SER   206      31.185  27.304  18.364  1.00 45.40
ATOM   1552  N   CYS   207      30.260  29.291  17.894  1.00 46.32
ATOM   1553  CA  CYS   207      28.912  28.764  18.079  1.00 48.14
ATOM   1554  CB  CYS   207      27.869  29.842  17.780  1.00 46.74
ATOM   1555  SG  CYS   207      27.946  31.264  18.883  1.00 42.50
ATOM   1556  C   CYS   207      28.666  27.551  17.186  1.00 50.79
ATOM   1557  O   CYS   207      27.715  26.799  17.403  1.00 50.97
ATOM   1558  N   TYR   208      29.533  27.361  16.190  1.00 53.91
ATOM   1559  CA  TYR   208      29.418  26.243  15.247  1.00 56.61
ATOM   1560  CB  TYR   208      30.350  26.458  14.045  1.00 56.96
ATOM   1561  CG  TYR   208      30.370  25.303  13.062  1.00 57.29
ATOM   1562  CD1 TYR   208      29.307  25.090  12.182  1.00 57.54
ATOM   1563  CE1 TYR   208      29.319  24.026  11.280  1.00 57.47
ATOM   1564  CD2 TYR   208      31.448  24.418  13.019  1.00 57.54
ATOM   1565  CE2 TYR   208      31.468  23.350  12.125  1.00 57.60
ATOM   1566  CZ  TYR   208      30.404  23.163  11.258  1.00 57.47
ATOM   1567  OH  TYR   208      30.435  22.126  10.360  1.00 57.71
ATOM   1568  C   TYR   208      29.705  24.867  15.854  1.00 58.12
ATOM   1569  O   TYR   208      28.874  23.960  15.773  1.00 58.61
ATOM   1570  N   TYR   209      30.876  24.699  16.459  1.00 59.77
ATOM   1571  CA  TYR   209      31.198  23.399  17.028  1.00 61.36
ATOM   1572  CB  TYR   209      32.619  23.394  17.581  1.00 63.23
ATOM   1573  CG  TYR   209      33.648  23.401  16.472  1.00 65.26
ATOM   1574  CD1 TYR   209      34.058  24.595  15.876  1.00 66.13
ATOM   1575  CE1 TYR   209      34.959  24.594  14.807  1.00 67.31
ATOM   1576  CD2 TYR   209      34.165  22.206  15.973  1.00 65.88
ATOM   1577  CE2 TYR   209      35.062  22.193  14.906  1.00 66.79
ATOM   1578  CZ  TYR   209      35.457  23.386  14.328  1.00 67.37
ATOM   1579  OH  TYR   209      36.350  23.370  13.277  1.00 67.62
ATOM   1580  C   TYR   209      30.206  22.965  18.083  1.00 61.32
ATOM   1581  O   TYR   209      30.048  21.771  18.336  1.00 61.19
ATOM   1582  N   GLU   210      29.523  23.938  18.680  1.00 61.63
ATOM   1583  CA  GLU   210      28.524  23.658  19.701  1.00 61.05
ATOM   1584  CB  GLU   210      28.444  24.808  20.706  1.00 62.29
ATOM   1585  CG  GLU   210      27.539  24.499  21.884  1.00 65.45
ATOM   1586  CD  GLU   210      27.716  25.463  23.050  1.00 67.38
ATOM   1587  OE1 GLU   210      28.865  25.609  23.535  1.00 68.93
ATOM   1588  OE2 GLU   210      26.707  26.065  23.488  1.00 67.92
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Figure 4

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ATOM   1589  C   GLU  210      27.175  23.459  19.026  1.00 60.04
ATOM   1590  O   GLU  210      26.255  22.901  19.618  1.00 59.93
ATOM   1591  N   ASP  211      27.073  23.920  17.780  1.00 58.82
ATOM   1592  CA  ASP  211      25.849  23.797  16.984  1.00 57.80
ATOM   1593  CB  ASP  211      24.804  24.824  17.441  1.00 58.16
ATOM   1594  CG  ASP  211      23.504  24.730  16.653  1.00 58.25
ATOM   1595  OD1 ASP  211      22.490  25.299  17.111  1.00 57.88
ATOM   1596  OD2 ASP  211      23.495  24.096  15.572  1.00 58.65
ATOM   1597  C   ASP  211      26.173  23.993  15.503  1.00 56.54
ATOM   1598  O   ASP  211      26.351  25.116  15.037  1.00 56.17
ATOM   1599  N   HIS  212      26.234  22.884  14.773  1.00 55.81
ATOM   1600  CA  HIS  212      26.577  22.884  13.351  1.00 55.26
ATOM   1601  CB  HIS  212      26.699  21.442  12.852  1.00 57.87
ATOM   1602  CG  HIS  212      27.816  20.678  13.493  1.00 61.52
ATOM   1603  CD2 HIS  212      27.815  19.527  14.205  1.00 62.63
ATOM   1604  ND1 HIS  212      29.127  21.110  13.460  1.00 62.80
ATOM   1605  CE1 HIS  212      29.884  20.258  14.127  1.00 63.70
ATOM   1606  NE2 HIS  212      29.114  19.288  14.590  1.00 63.71
ATOM   1607  C   HIS  212      25.665  23.656  12.412  1.00 53.29
ATOM   1608  O   HIS  212      26.014  23.883  11.251  1.00 52.77
ATOM   1609  N   GLN  213      24.496  24.058  12.895  1.00 51.08
ATOM   1610  CA  GLN  213      23.579  24.790  12.037  1.00 48.22
ATOM   1611  CB  GLN  213      22.135  24.347  12.298  1.00 49.39
ATOM   1612  CG  GLN  213      21.957  22.839  12.130  1.00 50.76
ATOM   1613  CD  GLN  213      20.507  22.410  11.965  1.00 51.82
ATOM   1614  OE1 GLN  213      19.653  22.721  12.803  1.00 52.48
ATOM   1615  NE2 GLN  213      20.223  21.679  10.883  1.00 51.72
ATOM   1616  C   GLN  213      23.746  26.289  12.202  1.00 45.19
ATOM   1617  O   GLN  213      22.978  27.077  11.654  1.00 45.00
ATOM   1618  N   CYS  214      24.759  26.686  12.957  1.00 41.87
ATOM   1619  CA  CYS  214      25.015  28.105  13.122  1.00 39.08
ATOM   1620  CB  CYS  214      25.907  28.386  14.332  1.00 39.18
ATOM   1621  SG  CYS  214      26.281  30.175  14.542  1.00 40.32
ATOM   1622  C   CYS  214      25.743  28.530  11.859  1.00 36.43
ATOM   1623  O   CYS  214      26.915  28.214  11.689  1.00 36.06
ATOM   1624  N   GLU  215      25.046  29.223  10.967  1.00 33.00
ATOM   1625  CA  GLU  215      25.664  29.672   9.736  1.00 30.60
ATOM   1626  CB  GLU  215      25.056  28.960   8.541  1.00 31.95
ATOM   1627  CG  GLU  215      25.289  27.466   8.561  1.00 33.57
ATOM   1628  CD  GLU  215      24.973  26.827   7.233  1.00 35.80
ATOM   1629  OE1 GLU  215      25.719  27.094   6.264  1.00 37.32
ATOM   1630  OE2 GLU  215      23.978  26.064   7.156  1.00 37.21
ATOM   1631  C   GLU  215      25.518  31.162   9.563  1.00 28.84
ATOM   1632  O   GLU  215      25.665  31.687   8.459  1.00 28.39
ATOM   1633  N   VAL  216      25.243  31.847  10.669  1.00 26.45
ATOM   1634  CA  VAL  216      25.083  33.291  10.648  1.00 23.67
ATOM   1635  CB  VAL  216      23.589  33.706  10.607  1.00 23.44
ATOM   1636  CG1 VAL  216      23.485  35.214  10.492  1.00 22.72
ATOM   1637  CG2 VAL  216      22.875  33.031   9.449  1.00 22.30
ATOM   1638  C   VAL  216      25.671  33.858  11.921  1.00 22.20
ATOM   1639  O   VAL  216      25.444  33.328  13.006  1.00 22.86
ATOM   1640  N   GLY  217      26.423  34.939  11.793  1.00 21.40
ATOM   1641  CA  GLY  217      26.997  35.554  12.965  1.00 21.14
ATOM   1642  C   GLY  217      26.524  36.994  13.022  1.00 22.30
ATOM   1643  O   GLY  217      26.432  37.677  11.983  1.00 22.05
ATOM   1644  N   MSE  218      26.201  37.454  14.228  1.00 23.03
ATOM   1645  CA  MSE  218      25.748  38.815  14.414  1.00 23.03
ATOM   1646  CB  MSE  218      24.208  38.880  14.445  1.00 25.98
ATOM   1647  CG  MSE  218      23.647  40.306  14.646  1.00 28.99
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Figure 4

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ATOM   1648  SE  MSE   218      21.806  40.486  14.543  1.00 35.34
ATOM   1649  CE  MSE   218      21.273  39.804  16.207  1.00 31.95
ATOM   1650  C   MSE   218      26.320  39.405  15.694  1.00 21.99
ATOM   1651  O   MSE   218      26.425  38.738  16.724  1.00 22.34
ATOM   1652  N   ILE   219      26.694  40.670  15.606  1.00 21.28
ATOM   1653  CA  ILE   219      27.240  41.402  16.720  1.00 20.85
ATOM   1654  CB  ILE   219      28.702  41.840  16.449  1.00 20.74
ATOM   1655  CG2 ILE   219      29.164  42.757  17.558  1.00 19.65
ATOM   1656  CG1 ILE   219      29.623  40.627  16.335  1.00 19.32
ATOM   1657  CD1 ILE   219      29.656  39.770  17.596  1.00 20.63
ATOM   1658  C   ILE   219      26.413  42.676  16.838  1.00 21.47
ATOM   1659  O   ILE   219      26.297  43.431  15.868  1.00 21.30
ATOM   1660  N   VAL   220      25.823  42.908  18.003  1.00 21.91
ATOM   1661  CA  VAL   220      25.059  44.135  18.224  1.00 22.49
ATOM   1662  CB  VAL   220      23.563  43.873  18.479  1.00 22.04
ATOM   1663  CG1 VAL   220      22.815  45.183  18.425  1.00 21.50
ATOM   1664  CG2 VAL   220      23.007  42.901  17.463  1.00 22.03
ATOM   1665  C   VAL   220      25.650  44.775  19.477  1.00 23.27
ATOM   1666  O   VAL   220      25.095  44.642  20.575  1.00 23.94
ATOM   1667  N   GLY   221      26.795  45.436  19.312  1.00 22.78
ATOM   1668  CA  GLY   221      27.448  46.063  20.443  1.00 22.86
ATOM   1669  C   GLY   221      27.728  47.509  20.138  1.00 23.75
ATOM   1670  O   GLY   221      26.816  48.264  19.828  1.00 25.09
ATOM   1671  N   THR   222      28.988  47.906  20.233  1.00 24.06
ATOM   1672  CA  THR   222      29.375  49.277  19.939  1.00 24.06
ATOM   1673  CB  THR   222      30.893  49.423  19.960  1.00 24.59
ATOM   1674  OG1 THR   222      31.377  49.051  21.258  1.00 26.00
ATOM   1675  CG2 THR   222      31.299  50.860  19.640  1.00 24.67
ATOM   1676  C   THR   222      28.888  49.530  18.533  1.00 24.09
ATOM   1677  O   THR   222      28.248  50.530  18.259  1.00 24.72
ATOM   1678  N   GLY   223      29.211  48.597  17.646  1.00 24.40
ATOM   1679  CA  GLY   223      28.790  48.686  16.262  1.00 24.65
ATOM   1680  C   GLY   223      27.797  47.560  16.020  1.00 25.05
ATOM   1681  O   GLY   223      27.478  46.779  16.936  1.00 25.80
ATOM   1682  N   CYS   224      27.298  47.453  14.798  1.00 24.73
ATOM   1683  CA  CYS   224      26.338  46.405  14.504  1.00 24.18
ATOM   1684  CB  CYS   224      24.928  46.958  14.682  1.00 24.47
ATOM   1685  SG  CYS   224      23.640  45.925  13.998  1.00 25.11
ATOM   1686  C   CYS   224      26.550  45.895  13.085  1.00 23.65
ATOM   1687  O   CYS   224      26.618  46.683  12.144  1.00 24.07
ATOM   1688  N   ASN   225      26.650  44.578  12.941  1.00 23.06
ATOM   1689  CA  ASN   225      26.883  43.963  11.638  1.00 23.27
ATOM   1690  CB  ASN   225      28.346  44.230  11.210  1.00 26.15
ATOM   1691  CG  ASN   225      28.831  43.296  10.098  1.00 27.94
ATOM   1692  OD1 ASN   225      28.271  43.265   8.997  1.00 29.23
ATOM   1693  ND2 ASN   225      29.878  42.524  10.393  1.00 28.62
ATOM   1694  C   ASN   225      26.603  42.459  11.740  1.00 21.80
ATOM   1695  O   ASN   225      26.291  41.954  12.827  1.00 20.54
ATOM   1696  N   ALA   226      26.709  41.759  10.610  1.00 19.99
ATOM   1697  CA  ALA   226      26.478  40.322  10.566  1.00 19.47
ATOM   1698  CB  ALA   226      24.994  40.032  10.443  1.00 20.99
ATOM   1699  C   ALA   226      27.194  39.723   9.378  1.00 18.72
ATOM   1700  O   ALA   226      27.529  40.428   8.415  1.00 17.97
ATOM   1701  N   CYS   227      27.404  38.415   9.439  1.00 18.36
ATOM   1702  CA  CYS   227      28.077  37.675   8.368  1.00 19.35
ATOM   1703  CB  CYS   227      29.523  37.396   8.751  1.00 18.42
ATOM   1704  SG  CYS   227      29.556  36.326  10.207  1.00 20.13
ATOM   1705  C   CYS   227      27.331  36.352   8.291  1.00 19.81
ATOM   1706  O   CYS   227      26.702  35.951   9.280  1.00 20.62
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Figure 4

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ATOM   1707  N   TYR   228      27.402  35.668   7.148  1.00 20.49
ATOM   1708  CA  TYR   228      26.705  34.384   6.989  1.00 20.56
ATOM   1709  CB  TYR   228      25.242  34.633   6.624  1.00 17.90
ATOM   1710  CG  TYR   228      25.096  35.134   5.204  1.00 15.65
ATOM   1711  CD1 TYR   228      24.922  34.249   4.145  1.00 15.81
ATOM   1712  CE1 TYR   228      24.885  34.701   2.823  1.00 15.89
ATOM   1713  CD2 TYR   228      25.221  36.483   4.913  1.00 15.28
ATOM   1714  CE2 TYR   228      25.186  36.949   3.601  1.00 16.08
ATOM   1715  CZ  TYR   228      25.022  36.051   2.564  1.00 16.76
ATOM   1716  OH  TYR   228      25.033  36.505   1.263  1.00 18.93
ATOM   1717  C   TYR   228      27.345  33.539   5.887  1.00 22.19
ATOM   1718  O   TYR   228      28.174  34.024   5.112  1.00 21.49
ATOM   1719  N   MSE   229      26.928  32.278   5.808  1.00 24.74
ATOM   1720  CA  MSE   229      27.438  31.349   4.808  1.00 26.69
ATOM   1721  CB  MSE   229      27.342  29.918   5.339  1.00 28.61
ATOM   1722  CG  MSE   229      28.167  29.637   6.598  1.00 32.37
ATOM   1723  SE  MSE   229      29.987  30.056   6.460  1.00 41.17
ATOM   1724  CE  MSE   229      30.544  28.874   5.098  1.00 36.30
ATOM   1725  C   MSE   229      26.663  31.470   3.481  1.00 27.83
ATOM   1726  O   MSE   229      25.535  30.994   3.363  1.00 28.02
ATOM   1727  N   GLU   230      27.282  32.109   2.492  1.00 29.19
ATOM   1728  CA  GLU   230      26.688  32.296   1.172  1.00 29.81
ATOM   1729  CB  GLU   230      27.165  33.623   0.577  1.00 30.83
ATOM   1730  CG  GLU   230      26.685  33.922  -0.843  1.00 32.33
ATOM   1731  CD  GLU   230      25.173  33.825  -0.989  1.00 34.04
ATOM   1732  OE1 GLU   230      24.663  32.698  -1.222  1.00 34.43
ATOM   1733  OE2 GLU   230      24.497  34.878  -0.858  1.00 33.65
ATOM   1734  C   GLU   230      27.127  31.143   0.282  1.00 30.91
ATOM   1735  O   GLU   230      27.958  30.319   0.685  1.00 30.80
ATOM   1736  N   GLU   231      26.562  31.078  -0.923  1.00 32.47
ATOM   1737  CA  GLU   231      26.885  30.024  -1.883  1.00 34.04
ATOM   1738  CB  GLU   231      25.668  29.696  -2.745  1.00 34.21
ATOM   1739  CG  GLU   231      24.408  29.396  -1.979  1.00 34.89
ATOM   1740  CD  GLU   231      24.452  28.054  -1.296  1.00 36.36
ATOM   1741  OE1 GLU   231      24.745  27.064  -2.002  1.00 36.80
ATOM   1742  OE2 GLU   231      24.182  27.981  -0.067  1.00 36.72
ATOM   1743  C   GLU   231      27.997  30.550  -2.777  1.00 35.65
ATOM   1744  O   GLU   231      27.889  31.663  -3.304  1.00 35.42
ATOM   1745  N   MSE   232      29.060  29.758  -2.952  1.00 37.13
ATOM   1746  CA  MSE   232      30.188  30.181  -3.780  1.00 38.19
ATOM   1747  CB  MSE   232      31.191  29.036  -3.935  1.00 41.27
ATOM   1748  CG  MSE   232      32.195  28.912  -2.765  1.00 45.40
ATOM   1749  SE  MSE   232      33.237  30.431  -2.467  1.00 52.07
ATOM   1750  CE  MSE   232      34.286  30.483  -3.969  1.00 48.20
ATOM   1751  C   MSE   232      29.694  30.664  -5.137  1.00 38.02
ATOM   1752  O   MSE   232      30.179  31.656  -5.678  1.00 36.84
ATOM   1753  N   GLN   233      28.698  29.970  -5.668  1.00 38.35
ATOM   1754  CA  GLN   233      28.110  30.331  -6.948  1.00 38.79
ATOM   1755  CB  GLN   233      26.954  29.373  -7.257  1.00 40.19
ATOM   1756  CG  GLN   233      25.658  30.041  -7.672  1.00 41.80
ATOM   1757  CD  GLN   233      24.460  29.119  -7.510  1.00 43.22
ATOM   1758  OE1 GLN   233      24.226  28.582  -6.424  1.00 44.27
ATOM   1759  NE2 GLN   233      23.688  28.936  -8.586  1.00 43.87
ATOM   1760  C   GLN   233      27.615  31.777  -6.936  1.00 38.45
ATOM   1761  O   GLN   233      27.495  32.407  -7.984  1.00 39.07
ATOM   1762  N   ASN   234      27.329  32.313  -5.753  1.00 37.79
ATOM   1763  CA  ASN   234      26.840  33.687  -5.668  1.00 36.56
ATOM   1764  CB  ASN   234      25.657  33.771  -4.706  1.00 37.03
ATOM   1765  CG  ASN   234      24.505  32.864  -5.119  1.00 36.83
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Figure 4

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ATOM   1766  OD1 ASN   234      24.152  32.793  -6.299  1.00 36.50
ATOM   1767  ND2 ASN   234      23.910  32.173  -4.146  1.00 36.25
ATOM   1768  C   ASN   234      27.919  34.676  -5.250  1.00 35.71
ATOM   1769  O   ASN   234      27.712  35.890  -5.301  1.00 35.11
ATOM   1770  N   VAL   235      29.069  34.156  -4.837  1.00 35.22
ATOM   1771  CA  VAL   235      30.177  35.009  -4.439  1.00 34.85
ATOM   1772  CB  VAL   235      31.056  34.321  -3.384  1.00 34.01
ATOM   1773  CG1 VAL   235      31.949  35.343  -2.717  1.00 32.35
ATOM   1774  CG2 VAL   235      30.185  33.576  -2.376  1.00 32.63
ATOM   1775  C   VAL   235      30.999  35.209  -5.706  1.00 35.79
ATOM   1776  O   VAL   235      32.011  34.548  -5.910  1.00 35.65
ATOM   1777  N   GLU   236      30.556  36.125  -6.556  1.00 37.55
ATOM   1778  CA  GLU   236      31.220  36.383  -7.830  1.00 39.52
ATOM   1779  CB  GLU   236      30.337  37.284  -8.701  1.00 39.67
ATOM   1780  CG  GLU   236      29.242  36.539  -9.448  1.00 41.02
ATOM   1781  CD  GLU   236      28.214  37.467 -10.072  1.00 42.58
ATOM   1782  OE1 GLU   236      28.607  38.529 -10.630  1.00 42.67
ATOM   1783  OE2 GLU   236      27.009  37.121 -10.011  1.00 43.02
ATOM   1784  C   GLU   236      32.631  36.961  -7.782  1.00 40.97
ATOM   1785  O   GLU   236      33.328  36.967  -8.803  1.00 42.27
ATOM   1786  N   LEU   237      33.064  37.457  -6.628  1.00 41.32
ATOM   1787  CA  LEU   237      34.408  38.017  -6.538  1.00 41.63
ATOM   1788  CB  LEU   237      34.438  39.163  -5.537  1.00 41.68
ATOM   1789  CG  LEU   237      33.545  40.367  -5.820  1.00 42.50
ATOM   1790  CD1 LEU   237      33.630  41.301  -4.623  1.00 44.17
ATOM   1791  CD2 LEU   237      33.984  41.101  -7.085  1.00 42.46
ATOM   1792  C   LEU   237      35.454  36.970  -6.148  1.00 42.43
ATOM   1793  O   LEU   237      36.636  37.294  -6.010  1.00 42.30
ATOM   1794  N   VAL   238      35.019  35.724  -5.967  1.00 42.96
ATOM   1795  CA  VAL   238      35.922  34.629  -5.606  1.00 43.89
ATOM   1796  CB  VAL   238      35.917  34.380  -4.097  1.00 42.33
ATOM   1797  CG1 VAL   238      36.722  33.136  -3.769  1.00 41.32
ATOM   1798  CG2 VAL   238      36.503  35.578  -3.385  1.00 42.74
ATOM   1799  C   VAL   238      35.520  33.337  -6.313  1.00 45.65
ATOM   1800  O   VAL   238      34.755  32.555  -5.770  1.00 46.15
ATOM   1801  N   GLU   239      36.069  33.116  -7.510  1.00 47.60
ATOM   1802  CA  GLU   239      35.769  31.947  -8.346  1.00 48.96
ATOM   1803  CB  GLU   239      36.819  31.793  -9.448  1.00 51.17
ATOM   1804  CG  GLU   239      37.000  33.026 -10.290  1.00 53.95
ATOM   1805  CD  GLU   239      37.817  34.066  -9.570  1.00 56.27
ATOM   1806  OE1 GLU   239      39.070  33.982  -9.637  1.00 58.40
ATOM   1807  OE2 GLU   239      37.211  34.950  -8.918  1.00 57.25
ATOM   1808  C   GLU   239      35.599  30.594  -7.675  1.00 48.87
ATOM   1809  O   GLU   239      36.272  30.274  -6.701  1.00 48.25
ATOM   1810  N   GLY   240      34.705  29.797  -8.252  1.00 49.09
ATOM   1811  CA  GLY   240      34.412  28.469  -7.750  1.00 50.05
ATOM   1812  C   GLY   240      32.967  28.418  -7.296  1.00 51.04
ATOM   1813  O   GLY   240      32.482  29.379  -6.712  1.00 52.00
ATOM   1814  N   ASP   241      32.259  27.332  -7.580  1.00 51.38
ATOM   1815  CA  ASP   241      30.882  27.214  -7.127  1.00 52.10
ATOM   1816  CB  ASP   241      29.963  26.766  -8.252  1.00 52.95
ATOM   1817  CG  ASP   241      30.186  27.534  -9.529  1.00 53.84
ATOM   1818  OD1 ASP   241      30.046  28.779  -9.522  1.00 53.20
ATOM   1819  OD2 ASP   241      30.496  26.875 -10.546  1.00 53.97
ATOM   1820  C   ASP   241      30.924  26.122  -6.083  1.00 52.90
ATOM   1821  O   ASP   241      29.898  25.563  -5.701  1.00 53.59
ATOM   1822  N   GLU   242      32.131  25.816  -5.626  1.00 53.45
ATOM   1823  CA  GLU   242      32.325  24.760  -4.646  1.00 53.65
ATOM   1824  CB  GLU   242      33.785  24.299  -4.670  1.00 55.19
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Figure 4

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ATOM   1825  CG  GLU  242      34.056  23.062  -3.826  1.00 57.57
ATOM   1826  CD  GLU  242      35.527  22.672  -3.811  1.00 58.85
ATOM   1827  OE1 GLU  242      36.063  22.340  -4.893  1.00 59.63
ATOM   1828  OE2 GLU  242      36.143  22.701  -2.717  1.00 59.85
ATOM   1829  C   GLU  242      31.933  25.159  -3.229  1.00 52.66
ATOM   1830  O   GLU  242      32.469  26.113  -2.661  1.00 53.15
ATOM   1831  N   GLY  243      30.987  24.418  -2.665  1.00 51.11
ATOM   1832  CA  GLY  243      30.545  24.673  -1.305  1.00 48.74
ATOM   1833  C   GLY  243      30.200  26.110  -0.967  1.00 46.87
ATOM   1834  O   GLY  243      29.879  26.917  -1.850  1.00 46.49
ATOM   1835  N   ARG  244      30.288  26.421   0.326  1.00 44.89
ATOM   1836  CA  ARG  244      29.967  27.748   0.838  1.00 43.27
ATOM   1837  CB  ARG  244      28.852  27.639   1.873  1.00 42.24
ATOM   1838  CG  ARG  244      27.571  27.040   1.339  1.00 42.16
ATOM   1839  CD  ARG  244      26.442  27.153   2.356  1.00 41.95
ATOM   1840  NE  ARG  244      25.254  26.425   1.925  1.00 39.30
ATOM   1841  CZ  ARG  244      24.702  25.446   2.630  1.00 39.15
ATOM   1842  NH1 ARG  244      25.236  25.085   3.794  1.00 38.10
ATOM   1843  NH2 ARG  244      23.627  24.821   2.168  1.00 38.77
ATOM   1844  C   ARG  244      31.121  28.524   1.465  1.00 42.34
ATOM   1845  O   ARG  244      32.089  27.945   1.958  1.00 41.77
ATOM   1846  N   MSE  245      30.990  29.849   1.446  1.00 42.07
ATOM   1847  CA  MSE  245      31.977  30.745   2.042  1.00 41.32
ATOM   1848  CB  MSE  245      32.846  31.391   0.974  1.00 42.25
ATOM   1849  CG  MSE  245      33.870  32.345   1.566  1.00 44.07
ATOM   1850  SE  MSE  245      34.884  33.206   0.332  1.00 47.16
ATOM   1851  CE  MSE  245      36.149  31.909  -0.005  1.00 44.40
ATOM   1852  C   MSE  245      31.324  31.863   2.863  1.00 40.37
ATOM   1853  O   MSE  245      30.525  32.644   2.338  1.00 40.13
ATOM   1854  N   CYS  246      31.664  31.940   4.148  1.00 38.95
ATOM   1855  CA  CYS  246      31.125  32.990   5.001  1.00 37.00
ATOM   1856  CB  CYS  246      31.794  32.953   6.376  1.00 37.69
ATOM   1857  SG  CYS  246      31.231  34.229   7.567  1.00 38.96
ATOM   1858  C   CYS  246      31.422  34.320   4.311  1.00 35.82
ATOM   1859  O   CYS  246      32.484  34.497   3.706  1.00 34.54
ATOM   1860  N   VAL  247      30.466  35.240   4.388  1.00 34.51
ATOM   1861  CA  VAL  247      30.591  36.566   3.782  1.00 32.46
ATOM   1862  CB  VAL  247      29.609  36.751   2.588  1.00 32.34
ATOM   1863  CG1 VAL  247      29.709  38.170   2.038  1.00 31.78
ATOM   1864  CG2 VAL  247      29.930  35.750   1.486  1.00 32.04
ATOM   1865  C   VAL  247      30.239  37.580   4.863  1.00 32.03
ATOM   1866  O   VAL  247      29.291  37.377   5.628  1.00 33.28
ATOM   1867  N   ASN  248      31.011  38.657   4.931  1.00 29.34
ATOM   1868  CA  ASN  248      30.792  39.699   5.917  1.00 27.36
ATOM   1869  CB  ASN  248      32.147  40.219   6.401  1.00 28.42
ATOM   1870  CG  ASN  248      32.031  41.471   7.253  1.00 29.34
ATOM   1871  OD1 ASN  248      30.975  41.774   7.816  1.00 29.82
ATOM   1872  ND2 ASN  248      33.141  42.201   7.374  1.00 29.54
ATOM   1873  C   ASN  248      29.983  40.798   5.257  1.00 27.10
ATOM   1874  O   ASN  248      30.531  41.618   4.503  1.00 26.98
ATOM   1875  N   THR  249      28.679  40.823   5.544  1.00 26.01
ATOM   1876  CA  THR  249      27.778  41.809   4.937  1.00 23.85
ATOM   1877  CB  THR  249      26.325  41.634   5.424  1.00 23.81
ATOM   1878  OG1 THR  249      26.228  42.100   6.775  1.00 25.10
ATOM   1879  CG2 THR  249      25.899  40.156   5.380  1.00 22.15
ATOM   1880  C   THR  249      28.208  43.226   5.270  1.00 24.20
ATOM   1881  O   THR  249      28.023  44.143   4.467  1.00 23.38
ATOM   1882  N   GLU  250      28.777  43.406   6.462  1.00 24.31
ATOM   1883  CA  GLU  250      29.219  44.733   6.891  1.00 23.61
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Figure 4

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ATOM   1884  CB  GLU  250      30.446  45.145   6.060  1.00 23.87
ATOM   1885  CG  GLU  250      31.242  46.362   6.571  1.00 25.94
ATOM   1886  CD  GLU  250      32.237  46.041   7.700  1.00 25.83
ATOM   1887  OE1 GLU  250      32.728  44.893   7.813  1.00 25.67
ATOM   1888  OE2 GLU  250      32.552  46.960   8.473  1.00 26.46
ATOM   1889  C   GLU  250      28.003  45.624   6.589  1.00 23.30
ATOM   1890  O   GLU  250      28.110  46.648   5.896  1.00 23.33
ATOM   1891  N   TRP  251      26.841  45.208   7.096  1.00 22.28
ATOM   1892  CA  TRP  251      25.609  45.940   6.840  1.00 22.36
ATOM   1893  CB  TRP  251      24.376  45.077   7.133  1.00 20.65
ATOM   1894  CG  TRP  251      24.133  44.726   8.543  1.00 18.29
ATOM   1895  CD2 TRP  251      23.308  43.648   9.016  1.00 16.51
ATOM   1896  CE2 TRP  251      23.279  43.725  10.424  1.00 15.08
ATOM   1897  CE3 TRP  251      22.589  42.635   8.384  1.00 16.17
ATOM   1898  CD1 TRP  251      24.565  45.395   9.652  1.00 17.71
ATOM   1899  NE1 TRP  251      24.051  44.795  10.795  1.00 17.10
ATOM   1900  CZ2 TRP  251      22.567  42.830  11.201  1.00 14.23
ATOM   1901  CZ3 TRP  251      21.872  41.737   9.171  1.00 15.72
ATOM   1902  CH2 TRP  251      21.869  41.842  10.559  1.00 14.23
ATOM   1903  C   TRP  251      25.445  47.283   7.523  1.00 23.49
ATOM   1904  O   TRP  251      24.541  48.044   7.167  1.00 23.95
ATOM   1905  N   GLY  252      26.302  47.579   8.500  1.00 24.44
ATOM   1906  CA  GLY  252      26.214  48.857   9.179  1.00 25.17
ATOM   1907  C   GLY  252      26.195  49.979   8.152  1.00 26.19
ATOM   1908  O   GLY  252      25.715  51.086   8.429  1.00 26.19
ATOM   1909  N   ALA  253      26.714  49.675   6.960  1.00 26.83
ATOM   1910  CA  ALA  253      26.791  50.622   5.851  1.00 27.86
ATOM   1911  CB  ALA  253      27.822  50.148   4.851  1.00 27.90
ATOM   1912  C   ALA  253      25.448  50.834   5.144  1.00 28.52
ATOM   1913  O   ALA  253      25.249  51.834   4.448  1.00 27.73
ATOM   1914  N   PHE  254      24.536  49.884   5.314  1.00 30.23
ATOM   1915  CA  PHE  254      23.224  49.974   4.696  1.00 31.42
ATOM   1916  CB  PHE  254      22.289  48.947   5.314  1.00 31.71
ATOM   1917  CG  PHE  254      20.899  48.995   4.768  1.00 31.90
ATOM   1918  CD1 PHE  254      20.655  48.736   3.429  1.00 31.47
ATOM   1919  CD2 PHE  254      19.824  49.273   5.600  1.00 32.95
ATOM   1920  CE1 PHE  254      19.367  48.746   2.927  1.00 31.38
ATOM   1921  CE2 PHE  254      18.518  49.285   5.096  1.00 32.69
ATOM   1922  CZ  PHE  254      18.295  49.021   3.763  1.00 31.47
ATOM   1923  C   PHE  254      22.664  51.367   4.928  1.00 32.56
ATOM   1924  O   PHE  254      22.638  51.839   6.064  1.00 33.19
ATOM   1925  N   GLY  255      22.227  52.017   3.849  1.00 33.62
ATOM   1926  CA  GLY  255      21.674  53.354   3.947  1.00 34.98
ATOM   1927  C   GLY  255      22.673  54.429   3.565  1.00 36.85
ATOM   1928  O   GLY  255      22.317  55.604   3.424  1.00 36.70
ATOM   1929  N   ASP  256      23.932  54.038   3.395  1.00 38.95
ATOM   1930  CA  ASP  256      24.966  55.000   3.038  1.00 41.47
ATOM   1931  CB  ASP  256      26.349  54.347   3.088  1.00 41.77
ATOM   1932  CG  ASP  256      26.880  54.224   4.502  1.00 42.36
ATOM   1933  OD1 ASP  256      26.573  55.120   5.322  1.00 43.08
ATOM   1934  OD2 ASP  256      27.617  53.251   4.791  1.00 42.28
ATOM   1935  C   ASP  256      24.744  55.636   1.666  1.00 43.10
ATOM   1936  O   ASP  256      25.489  56.533   1.261  1.00 44.08
ATOM   1937  N   SER  257      23.729  55.171   0.946  1.00 44.19
ATOM   1938  CA  SER  257      23.427  55.738  -0.363  1.00 45.32
ATOM   1939  CB  SER  257      23.714  54.713  -1.467  1.00 45.78
ATOM   1940  OG  SER  257      22.845  53.601  -1.375  1.00 46.48
ATOM   1941  C   SER  257      21.967  56.204  -0.423  1.00 45.41
ATOM   1942  O   SER  257      21.378  56.316  -1.501  1.00 46.14
```

Figure 4


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ATOM   1943  N   GLY  258     21.393  56.466   0.751  1.00 45.52
ATOM   1944  CA  GLY  258     20.018  56.933   0.835  1.00 45.22
ATOM   1945  C   GLY  258     18.922  55.896   1.042  1.00 45.11
ATOM   1946  O   GLY  258     17.745  56.253   1.068  1.00 45.45
ATOM   1947  N   GLU  259     19.284  54.627   1.205  1.00 44.67
ATOM   1948  CA  GLU  259     18.288  53.572   1.380  1.00 44.04
ATOM   1949  CB  GLU  259     18.954  52.187   1.415  1.00 44.23
ATOM   1950  CG  GLU  259     19.952  51.916   0.295  1.00 44.88
ATOM   1951  CD  GLU  259     21.318  52.552   0.548  1.00 45.53
ATOM   1952  OE1 GLU  259     21.381  53.785   0.753  1.00 44.98
ATOM   1953  OE2 GLU  259     22.335  51.817   0.537  1.00 45.95
ATOM   1954  C   GLU  259     17.462  53.749   2.647  1.00 43.91
ATOM   1955  O   GLU  259     16.461  53.061   2.836  1.00 43.49
ATOM   1956  N   LEU  260     17.875  54.661   3.520  1.00 43.87
ATOM   1957  CA  LEU  260     17.143  54.865   4.765  1.00 44.40
ATOM   1958  CB  LEU  260     18.023  54.513   5.967  1.00 44.36
ATOM   1959  CG  LEU  260     18.398  53.041   6.153  1.00 44.87
ATOM   1960  CD1 LEU  260     19.315  52.879   7.369  1.00 44.30
ATOM   1961  CD2 LEU  260     17.127  52.216   6.307  1.00 44.88
ATOM   1962  C   LEU  260     16.632  56.282   4.932  1.00 44.59
ATOM   1963  O   LEU  260     15.744  56.534   5.749  1.00 44.72
ATOM   1964  N   ASP  261     17.200  57.202   4.161  1.00 44.48
ATOM   1965  CA  ASP  261     16.821  58.608   4.234  1.00 44.18
ATOM   1966  CB  ASP  261     16.813  59.224   2.841  1.00 44.99
ATOM   1967  CG  ASP  261     18.192  59.310   2.247  1.00 46.23
ATOM   1968  OD1 ASP  261     19.165  58.994   2.980  1.00 46.42
ATOM   1969  OD2 ASP  261     18.296  59.697   1.055  1.00 46.79
ATOM   1970  C   ASP  261     15.482  58.885   4.892  1.00 43.00
ATOM   1971  O   ASP  261     15.415  59.592   5.898  1.00 42.63
ATOM   1972  N   GLU  262     14.424  58.317   4.320  1.00 41.88
ATOM   1973  CA  GLU  262     13.070  58.525   4.810  1.00 41.00
ATOM   1974  CB  GLU  262     12.088  57.744   3.940  1.00 41.65
ATOM   1975  CG  GLU  262     12.249  56.254   3.999  1.00 43.54
ATOM   1976  CD  GLU  262     11.359  55.562   2.996  1.00 45.44
ATOM   1977  OE1 GLU  262     11.715  55.561   1.800  1.00 47.21
ATOM   1978  OE2 GLU  262     10.296  55.031   3.391  1.00 47.29
ATOM   1979  C   GLU  262     12.830  58.211   6.286  1.00 39.99
ATOM   1980  O   GLU  262     11.997  58.852   6.918  1.00 40.22
ATOM   1981  N   PHE  263     13.545  57.238   6.845  1.00 38.83
ATOM   1982  CA  PHE  263     13.360  56.908   8.258  1.00 37.00
ATOM   1983  CB  PHE  263     13.684  55.430   8.512  1.00 34.37
ATOM   1984  CG  PHE  263     12.828  54.476   7.717  1.00 32.41
ATOM   1985  CD1 PHE  263     13.366  53.753   6.660  1.00 30.67
ATOM   1986  CD2 PHE  263     11.474  54.317   8.012  1.00 30.95
ATOM   1987  CE1 PHE  263     12.567  52.886   5.909  1.00 29.82
ATOM   1988  CE2 PHE  263     10.667  53.450   7.261  1.00 28.87
ATOM   1989  CZ  PHE  263     11.214  52.737   6.213  1.00 29.09
ATOM   1990  C   PHE  263     14.197  57.797   9.190  1.00 36.78
ATOM   1991  O   PHE  263     13.809  58.041  10.327  1.00 37.58
ATOM   1992  N   LEU  264     15.328  58.301   8.712  1.00 36.72
ATOM   1993  CA  LEU  264     16.193  59.142   9.542  1.00 37.11
ATOM   1994  CB  LEU  264     17.389  59.638   8.725  1.00 36.98
ATOM   1995  CG  LEU  264     18.131  58.621   7.852  1.00 36.59
ATOM   1996  CD1 LEU  264     19.233  59.346   7.077  1.00 35.39
ATOM   1997  CD2 LEU  264     18.701  57.503   8.717  1.00 35.46
ATOM   1998  C   LEU  264     15.482  60.350  10.158  1.00 37.28
ATOM   1999  O   LEU  264     14.879  61.148   9.451  1.00 38.03
ATOM   2000  N   LEU  265     15.574  60.480  11.479  1.00 37.63
ATOM   2001  CA  LEU  265     14.965  61.585  12.215  1.00 37.33
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Figure 4

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ATOM   2002  CB  LEU  265      14.380  61.070  13.527  1.00 36.25
ATOM   2003  CG  LEU  265      13.529  59.807  13.417  1.00 35.76
ATOM   2004  CD1 LEU  265      13.157  59.295  14.808  1.00 35.17
ATOM   2005  CD2 LEU  265      12.292  60.120  12.598  1.00 35.59
ATOM   2006  C   LEU  265      16.054  62.613  12.521  1.00 38.22
ATOM   2007  O   LEU  265      17.239  62.285  12.486  1.00 38.34
ATOM   2008  N   GLU  266      15.653  63.844  12.832  1.00 39.22
ATOM   2009  CA  GLU  266      16.599  64.922  13.137  1.00 40.56
ATOM   2010  CB  GLU  266      15.874  66.101  13.813  1.00 41.82
ATOM   2011  CG  GLU  266      15.277  65.777  15.196  1.00 44.28
ATOM   2012  CD  GLU  266      14.612  66.974  15.886  1.00 44.95
ATOM   2013  OE1 GLU  266      13.543  67.432  15.410  1.00 45.08
ATOM   2014  OE2 GLU  266      15.163  67.452  16.910  1.00 45.53
ATOM   2015  C   GLU  266      17.733  64.435  14.036  1.00 40.54
ATOM   2016  O   GLU  266      18.910  64.657  13.750  1.00 40.69
ATOM   2017  N   TYR  267      17.366  63.760  15.121  1.00 40.61
ATOM   2018  CA  TYR  267      18.342  63.234  16.062  1.00 40.30
ATOM   2019  CB  TYR  267      17.639  62.364  17.110  1.00 39.44
ATOM   2020  CG  TYR  267      16.216  62.784  17.423  1.00 38.98
ATOM   2021  CD1 TYR  267      15.134  61.967  17.066  1.00 38.66
ATOM   2022  CE1 TYR  267      13.813  62.342  17.349  1.00 38.28
ATOM   2023  CD2 TYR  267      15.943  63.995  18.075  1.00 38.72
ATOM   2024  CE2 TYR  267      14.619  64.381  18.364  1.00 38.45
ATOM   2025  CZ  TYR  267      13.564  63.548  17.996  1.00 38.30
ATOM   2026  OH  TYR  267      12.267  63.923  18.251  1.00 37.22
ATOM   2027  C   TYR  267      19.381  62.403  15.296  1.00 40.27
ATOM   2028  O   TYR  267      20.580  62.469  15.579  1.00 40.14
ATOM   2029  N   ASP  268      18.909  61.626  14.324  1.00 40.61
ATOM   2030  CA  ASP  268      19.781  60.790  13.511  1.00 40.87
ATOM   2031  CB  ASP  268      18.946  59.920  12.566  1.00 39.36
ATOM   2032  CG  ASP  268      18.183  58.843  13.301  1.00 38.52
ATOM   2033  OD1 ASP  268      18.819  58.118  14.082  1.00 39.79
ATOM   2034  OD2 ASP  268      16.961  58.711  13.110  1.00 36.13
ATOM   2035  C   ASP  268      20.764  61.643  12.712  1.00 41.97
ATOM   2036  O   ASP  268      21.956  61.339  12.667  1.00 42.91
ATOM   2037  N   ARG  269      20.266  62.710  12.090  1.00 42.73
ATOM   2038  CA  ARG  269      21.113  63.606  11.310  1.00 43.23
ATOM   2039  CB  ARG  269      20.302  64.793  10.786  1.00 45.34
ATOM   2040  CG  ARG  269      18.923  64.464  10.223  1.00 47.46
ATOM   2041  CD  ARG  269      19.000  63.819   8.864  1.00 49.22
ATOM   2042  NE  ARG  269      17.667  63.552   8.337  1.00 52.67
ATOM   2043  CZ  ARG  269      17.426  62.969   7.165  1.00 54.63
ATOM   2044  NH1 ARG  269      18.436  62.591   6.386  1.00 55.41
ATOM   2045  NH2 ARG  269      16.173  62.747   6.775  1.00 55.38
ATOM   2046  C   ARG  269      22.204  64.150  12.231  1.00 42.99
ATOM   2047  O   ARG  269      23.400  63.999  11.977  1.00 43.63
ATOM   2048  N   LEU  270      21.777  64.796  13.305  1.00 41.99
ATOM   2049  CA  LEU  270      22.702  65.372  14.261  1.00 41.33
ATOM   2050  CB  LEU  270      21.924  65.812  15.502  1.00 41.15
ATOM   2051  CG  LEU  270      21.004  67.002  15.217  1.00 40.34
ATOM   2052  CD1 LEU  270      19.964  67.182  16.307  1.00 39.94
ATOM   2053  CD2 LEU  270      21.879  68.237  15.084  1.00 40.26
ATOM   2054  C   LEU  270      23.828  64.406  14.635  1.00 41.26
ATOM   2055  O   LEU  270      25.009  64.762  14.553  1.00 41.76
ATOM   2056  N   VAL  271      23.462  63.188  15.030  1.00 40.24
ATOM   2057  CA  VAL  271      24.443  62.177  15.415  1.00 40.08
ATOM   2058  CB  VAL  271      23.776  60.838  15.730  1.00 40.42
ATOM   2059  CG1 VAL  271      24.846  59.800  16.050  1.00 39.86
ATOM   2060  CG2 VAL  271      22.796  61.000  16.891  1.00 40.86
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	ATOM	2061	C	VAL	271	25.477	61.903	14.329	1.00	40.51
	ATOM	2062	O	VAL	271	26.676	61.832	14.595	1.00	40.15
	ATOM	2063	N	ASP	272	24.998	61.730	13.103	1.00	40.78
	ATOM	2064	CA	ASP	272	25.866	61.447	11.977	1.00	40.36
5	ATOM	2065	CB	ASP	272	25.038	61.344	10.695	1.00	39.16
	ATOM	2066	CG	ASP	272	25.792	60.670	9.553	1.00	38.09
	ATOM	2067	OD1	ASP	272	26.821	60.000	9.807	1.00	36.54
	ATOM	2068	OD2	ASP	272	25.335	60.798	8.394	1.00	37.12
	ATOM	2069	C	ASP	272	26.901	62.544	11.849	1.00	40.88
10	ATOM	2070	O	ASP	272	28.099	62.297	11.953	1.00	40.75
	ATOM	2071	N	GLU	273	26.429	63.763	11.638	1.00	41.96
	ATOM	2072	CA	GLU	273	27.321	64.896	11.477	1.00	43.14
	ATOM	2073	CB	GLU	273	26.501	66.170	11.470	1.00	44.13
	ATOM	2074	CG	GLU	273	25.576	66.214	10.272	1.00	46.73
15	ATOM	2075	CD	GLU	273	24.629	67.388	10.308	1.00	48.40
	ATOM	2076	OE1	GLU	273	25.047	68.455	10.828	1.00	49.15
	ATOM	2077	OE2	GLU	273	23.482	67.241	9.811	1.00	48.64
	ATOM	2078	C	GLU	273	28.428	64.968	12.517	1.00	43.48
	ATOM	2079	O	GLU	273	29.575	65.279	12.187	1.00	43.59
20	ATOM	2080	N	SER	274	28.095	64.666	13.767	1.00	44.05
	ATOM	2081	CA	SER	274	29.089	64.702	14.837	1.00	44.54
	ATOM	2082	CB	SER	274	28.421	64.568	16.205	1.00	45.39
	ATOM	2083	OG	SER	274	27.496	65.611	16.424	1.00	48.14
	ATOM	2084	C	SER	274	30.106	63.582	14.694	1.00	44.23
25	ATOM	2085	O	SER	274	31.292	63.783	14.931	1.00	44.76
	ATOM	2086	N	SER	275	29.632	62.400	14.318	1.00	43.84
	ATOM	2087	CA	SER	275	30.489	61.227	14.162	1.00	43.42
	ATOM	2088	CB	SER	275	29.754	60.139	13.392	1.00	43.28
	ATOM	2089	OG	SER	275	29.758	60.444	12.010	1.00	42.94
30	ATOM	2090	C	SER	275	31.789	61.535	13.426	1.00	43.34
	ATOM	2091	O	SER	275	31.914	62.552	12.738	1.00	43.76
	ATOM	2092	N	ALA	276	32.756	60.639	13.570	1.00	42.68
	ATOM	2093	CA	ALA	276	34.034	60.805	12.906	1.00	42.98
	ATOM	2094	CB	ALA	276	35.108	60.015	13.639	1.00	42.92
35	ATOM	2095	C	ALA	276	33.930	60.319	11.465	1.00	43.23
	ATOM	2096	O	ALA	276	34.936	60.277	10.751	1.00	44.60
	ATOM	2097	N	ASN	277	32.722	59.949	11.039	1.00	42.10
	ATOM	2098	CA	ASN	277	32.517	59.447	9.691	1.00	40.87
	ATOM	2099	CB	ASN	277	32.615	57.927	9.685	1.00	41.63
40	ATOM	2100	CG	ASN	277	31.654	57.283	10.659	1.00	42.64
	ATOM	2101	OD1	ASN	277	30.670	57.898	11.067	1.00	43.50
	ATOM	2102	ND2	ASN	277	31.925	56.033	11.029	1.00	42.98
	ATOM	2103	C	ASN	277	31.178	59.865	9.104	1.00	40.57
	ATOM	2104	O	ASN	277	30.430	59.039	8.579	1.00	39.89
45	ATOM	2105	N	PRO	278	30.868	61.163	9.163	1.00	40.83
	ATOM	2106	CD	PRO	278	31.783	62.282	9.451	1.00	40.90
	ATOM	2107	CA	PRO	278	29.600	61.657	8.623	1.00	40.71
	ATOM	2108	CB	PRO	278	29.807	63.175	8.579	1.00	40.88
	ATOM	2109	CG	PRO	278	31.303	63.326	8.474	1.00	41.27
50	ATOM	2110	C	PRO	278	29.239	61.074	7.258	1.00	40.60
	ATOM	2111	O	PRO	278	29.949	61.284	6.270	1.00	40.71
	ATOM	2112	N	GLY	279	28.131	60.338	7.216	1.00	40.34
	ATOM	2113	CA	GLY	279	27.676	59.747	5.971	1.00	39.10
	ATOM	2114	C	GLY	279	27.904	58.252	5.828	1.00	38.94
55	ATOM	2115	O	GLY	279	27.315	57.635	4.952	1.00	39.74
	ATOM	2116	N	GLN	280	28.735	57.660	6.683	1.00	38.66
	ATOM	2117	CA	GLN	280	29.049	56.230	6.605	1.00	37.75
	ATOM	2118	CB	GLN	280	30.563	56.043	6.513	1.00	37.97
	ATOM	2119	CG	GLN	280	31.243	56.954	5.509	1.00	39.85

Figure 4

ATOM	2120	CD	GLN	280	32.743	57.046	5.730	1.00	40.76
ATOM	2121	OE1	GLN	280	33.465	56.058	5.587	1.00	41.39
ATOM	2122	NE2	GLN	280	33.220	58.240	6.083	1.00	41.57
ATOM	2123	C	GLN	280	28.553	55.455	7.817	1.00	36.99
ATOM	2124	O	GLN	280	28.645	55.939	8.941	1.00	37.89
ATOM	2125	N	GLN	281	28.054	54.242	7.592	1.00	35.75
ATOM	2126	CA	GLN	281	27.572	53.401	8.681	1.00	34.04
ATOM	2127	CB	GLN	281	28.590	53.404	9.829	1.00	33.35
ATOM	2128	CG	GLN	281	29.971	52.951	9.447	1.00	33.09
ATOM	2129	CD	GLN	281	29.967	51.576	8.800	1.00	34.44
ATOM	2130	OE1	GLN	281	29.917	51.451	7.572	1.00	33.95
ATOM	2131	NE2	GLN	281	30.000	50.529	9.630	1.00	34.63
ATOM	2132	C	GLN	281	26.210	53.831	9.237	1.00	33.42
ATOM	2133	O	GLN	281	25.895	53.530	10.390	1.00	34.87
ATOM	2134	N	LEU	282	25.395	54.511	8.436	1.00	31.53
ATOM	2135	CA	LEU	282	24.098	54.992	8.913	1.00	29.87
ATOM	2136	CB	LEU	282	23.345	55.685	7.777	1.00	30.15
ATOM	2137	CG	LEU	282	24.030	56.871	7.085	1.00	30.41
ATOM	2138	CD1	LEU	282	22.963	57.741	6.435	1.00	29.82
ATOM	2139	CD2	LEU	282	24.815	57.699	8.097	1.00	30.66
ATOM	2140	C	LEU	282	23.191	53.949	9.578	1.00	28.70
ATOM	2141	O	LEU	282	22.716	54.153	10.698	1.00	28.78
ATOM	2142	N	TYR	283	22.935	52.841	8.894	1.00	27.35
ATOM	2143	CA	TYR	283	22.095	51.793	9.461	1.00	26.53
ATOM	2144	CB	TYR	283	22.233	50.511	8.633	1.00	24.41
ATOM	2145	CG	TYR	283	21.420	49.338	9.143	1.00	22.90
ATOM	2146	CD1	TYR	283	20.021	49.413	9.210	1.00	21.94
ATOM	2147	CE1	TYR	283	19.257	48.318	9.609	1.00	20.96
ATOM	2148	CD2	TYR	283	22.038	48.129	9.503	1.00	21.53
ATOM	2149	CE2	TYR	283	21.279	47.030	9.907	1.00	20.87
ATOM	2150	CZ	TYR	283	19.886	47.140	9.950	1.00	21.33
ATOM	2151	OH	TYR	283	19.105	46.068	10.310	1.00	23.85
ATOM	2152	C	TYR	283	22.567	51.532	10.891	1.00	27.12
ATOM	2153	O	TYR	283	21.783	51.521	11.841	1.00	28.95
ATOM	2154	N	GLU	284	23.869	51.352	11.035	1.00	26.60
ATOM	2155	CA	GLU	284	24.486	51.072	12.317	1.00	26.43
ATOM	2156	CB	GLU	284	25.982	50.905	12.108	1.00	27.03
ATOM	2157	CG	GLU	284	26.763	50.680	13.375	1.00	27.21
ATOM	2158	CD	GLU	284	28.224	50.492	13.082	1.00	27.57
ATOM	2159	OE1	GLU	284	28.897	51.506	12.734	1.00	27.02
ATOM	2160	OE2	GLU	284	28.670	49.319	13.185	1.00	26.30
ATOM	2161	C	GLU	284	24.249	52.133	13.381	1.00	26.81
ATOM	2162	O	GLU	284	24.197	51.826	14.582	1.00	26.06
ATOM	2163	N	LYS	285	24.134	53.384	12.940	1.00	27.07
ATOM	2164	CA	LYS	285	23.926	54.502	13.860	1.00	27.39
ATOM	2165	CB	LYS	285	24.339	55.825	13.186	1.00	25.99
ATOM	2166	CG	LYS	285	25.840	56.012	13.132	1.00	24.13
ATOM	2167	CD	LYS	285	26.235	57.110	12.179	1.00	23.29
ATOM	2168	CE	LYS	285	27.755	57.193	12.052	1.00	22.03
ATOM	2169	NZ	LYS	285	28.142	58.198	11.027	1.00	21.72
ATOM	2170	C	LYS	285	22.488	54.595	14.368	1.00	28.05
ATOM	2171	O	LYS	285	22.086	55.615	14.941	1.00	28.61
ATOM	2172	N	LEU	286	21.717	53.535	14.144	1.00	27.60
ATOM	2173	CA	LEU	286	20.335	53.488	14.599	1.00	27.30
ATOM	2174	CB	LEU	286	19.399	53.157	13.435	1.00	28.57
ATOM	2175	CG	LEU	286	19.375	54.167	12.279	1.00	30.25
ATOM	2176	CD1	LEU	286	18.480	53.647	11.139	1.00	29.98
ATOM	2177	CD2	LEU	286	18.863	55.507	12.780	1.00	29.35
ATOM	2178	C	LEU	286	20.260	52.381	15.632	1.00	27.01

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ATOM   2179  O   LEU  286      19.296  52.294  16.399  1.00 27.55
ATOM   2180  N   ILE  287      21.306  51.554  15.645  1.00 26.00
ATOM   2181  CA  ILE  287      21.415  50.399  16.532  1.00 24.38
ATOM   2182  CB  ILE  287      21.551  49.141  15.715  1.00 23.92
ATOM   2183  CG2 ILE  287      21.470  47.919  16.628  1.00 22.70
ATOM   2184  CG1 ILE  287      20.510  49.158  14.597  1.00 22.87
ATOM   2185  CD1 ILE  287      20.676  48.042  13.607  1.00 22.79
ATOM   2186  C   ILE  287      22.639  50.444  17.433  1.00 24.65
ATOM   2187  O   ILE  287      22.550  50.255  18.644  1.00 23.54
ATOM   2188  N   GLY  288      23.791  50.668  16.810  1.00 25.94
ATOM   2189  CA  GLY  288      25.060  50.714  17.519  1.00 26.86
ATOM   2190  C   GLY  288      25.081  51.266  18.927  1.00 27.76
ATOM   2191  O   GLY  288      24.697  52.412  19.164  1.00 28.19
ATOM   2192  N   GLY  289      25.554  50.445  19.860  1.00 28.95
ATOM   2193  CA  GLY  289      25.656  50.856  21.249  1.00 30.64
ATOM   2194  C   GLY  289      26.632  52.007  21.407  1.00 31.92
ATOM   2195  O   GLY  289      26.930  52.442  22.509  1.00 32.56
ATOM   2196  N   LYS  290      27.133  52.504  20.291  1.00 32.83
ATOM   2197  CA  LYS  290      28.067  53.607  20.296  1.00 33.99
ATOM   2198  CB  LYS  290      29.104  53.373  19.191  1.00 35.04
ATOM   2199  CG  LYS  290      29.858  54.598  18.665  1.00 36.71
ATOM   2200  CD  LYS  290      31.032  54.996  19.551  1.00 38.80
ATOM   2201  CE  LYS  290      31.936  56.011  18.839  1.00 39.77
ATOM   2202  NZ  LYS  290      32.864  56.707  19.787  1.00 41.04
ATOM   2203  C   LYS  290      27.278  54.880  20.035  1.00 34.58
ATOM   2204  O   LYS  290      27.810  55.984  20.138  1.00 35.79
ATOM   2205  N   TYR  291      26.001  54.734  19.708  1.00 33.80
ATOM   2206  CA  TYR  291      25.196  55.907  19.406  1.00 33.61
ATOM   2207  CB  TYR  291      25.010  56.046  17.892  1.00 33.22
ATOM   2208  CG  TYR  291      26.256  55.752  17.084  1.00 33.77
ATOM   2209  CD1 TYR  291      26.659  54.435  16.838  1.00 34.23
ATOM   2210  CE1 TYR  291      27.789  54.155  16.065  1.00 34.17
ATOM   2211  CD2 TYR  291      27.021  56.783  16.542  1.00 33.61
ATOM   2212  CE2 TYR  291      28.150  56.515  15.773  1.00 33.54
ATOM   2213  CZ  TYR  291      28.528  55.200  15.532  1.00 33.76
ATOM   2214  OH  TYR  291      29.620  54.928  14.729  1.00 34.36
ATOM   2215  C   TYR  291      23.836  55.874  20.070  1.00 33.11
ATOM   2216  O   TYR  291      23.069  56.828  19.975  1.00 32.86
ATOM   2217  N   MSE  292      23.521  54.778  20.737  1.00 33.27
ATOM   2218  CA  MSE  292      22.230  54.699  21.389  1.00 33.18
ATOM   2219  CB  MSE  292      22.066  53.349  22.062  1.00 33.77
ATOM   2220  CG  MSE  292      20.639  52.975  22.314  1.00 35.15
ATOM   2221  SE  MSE  292      20.564  51.230  22.803  1.00 41.54
ATOM   2222  CE  MSE  292      20.269  50.385  21.171  1.00 35.91
ATOM   2223  C   MSE  292      22.148  55.818  22.423  1.00 32.97
ATOM   2224  O   MSE  292      21.227  56.637  22.400  1.00 33.49
ATOM   2225  N   GLY  293      23.131  55.861  23.315  1.00 32.96
ATOM   2226  CA  GLY  293      23.151  56.892  24.334  1.00 32.25
ATOM   2227  C   GLY  293      23.067  58.290  23.750  1.00 32.18
ATOM   2228  O   GLY  293      22.307  59.126  24.241  1.00 33.24
ATOM   2229  N   GLU  294      23.835  58.560  22.702  1.00 31.47
ATOM   2230  CA  GLU  294      23.809  59.883  22.096  1.00 31.38
ATOM   2231  CB  GLU  294      24.875  59.971  21.008  1.00 33.29
ATOM   2232  CG  GLU  294      24.986  61.321  20.304  1.00 34.67
ATOM   2233  CD  GLU  294      25.227  62.474  21.257  1.00 35.80
ATOM   2234  OE1 GLU  294      25.708  62.244  22.389  1.00 36.49
ATOM   2235  OE2 GLU  294      24.946  63.623  20.858  1.00 37.16
ATOM   2236  C   GLU  294      22.428  60.192  21.521  1.00 30.62
ATOM   2237  O   GLU  294      21.919  61.305  21.664  1.00 30.94
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ATOM   2238  N   LEU  295      21.818  59.204  20.878  1.00 29.56
ATOM   2239  CA  LEU  295      20.495  59.392  20.303  1.00 29.24
ATOM   2240  CB  LEU  295      20.030  58.112  19.589  1.00 27.27
ATOM   2241  CG  LEU  295      20.389  58.007  18.099  1.00 25.46
ATOM   2242  CD1 LEU  295      19.979  56.668  17.522  1.00 21.87
ATOM   2243  CD2 LEU  295      19.677  59.136  17.352  1.00 25.71
ATOM   2244  C   LEU  295      19.497  59.787  21.388  1.00 29.98
ATOM   2245  O   LEU  295      18.587  60.573  21.156  1.00 30.19
ATOM   2246  N   VAL  296      19.665  59.250  22.585  1.00 31.23
ATOM   2247  CA  VAL  296      18.745  59.590  23.657  1.00 32.87
ATOM   2248  CB  VAL  296      18.890  58.623  24.831  1.00 32.48
ATOM   2249  CG1 VAL  296      17.827  58.899  25.868  1.00 32.99
ATOM   2250  CG2 VAL  296      18.762  57.198  24.323  1.00 33.56
ATOM   2251  C   VAL  296      19.020  61.025  24.122  1.00 33.74
ATOM   2252  O   VAL  296      18.086  61.778  24.431  1.00 33.68
ATOM   2253  N   ARG  297      20.296  61.409  24.145  1.00 34.02
ATOM   2254  CA  ARG  297      20.659  62.757  24.563  1.00 35.34
ATOM   2255  CB  ARG  297      22.147  63.008  24.342  1.00 34.89
ATOM   2256  CG  ARG  297      22.940  63.279  25.609  1.00 35.27
ATOM   2257  CD  ARG  297      23.791  64.525  25.454  1.00 35.98
ATOM   2258  NE  ARG  297      24.226  64.700  24.074  1.00 37.11
ATOM   2259  CZ  ARG  297      24.476  65.878  23.513  1.00 37.43
ATOM   2260  NH1 ARG  297      24.348  66.994  24.226  1.00 38.45
ATOM   2261  NH2 ARG  297      24.809  65.944  22.229  1.00 36.61
ATOM   2262  C   ARG  297      19.870  63.766  23.747  1.00 36.07
ATOM   2263  O   ARG  297      19.103  64.574  24.285  1.00 36.76
ATOM   2264  N   LEU  298      20.063  63.699  22.437  1.00 36.93
ATOM   2265  CA  LEU  298      19.407  64.596  21.500  1.00 37.55
ATOM   2266  CB  LEU  298      19.768  64.178  20.077  1.00 37.28
ATOM   2267  CG  LEU  298      21.272  64.065  19.816  1.00 36.13
ATOM   2268  CD1 LEU  298      21.478  63.784  18.341  1.00 36.85
ATOM   2269  CD2 LEU  298      21.991  65.356  20.218  1.00 35.02
ATOM   2270  C   LEU  298      17.892  64.633  21.670  1.00 38.53
ATOM   2271  O   LEU  298      17.276  65.708  21.618  1.00 38.44
ATOM   2272  N   VAL  299      17.289  63.462  21.866  1.00 39.23
ATOM   2273  CA  VAL  299      15.839  63.389  22.054  1.00 40.08
ATOM   2274  CB  VAL  299      15.349  61.932  22.110  1.00 39.44
ATOM   2275  CG1 VAL  299      13.844  61.892  22.385  1.00 37.91
ATOM   2276  CG2 VAL  299      15.676  61.240  20.802  1.00 38.72
ATOM   2277  C   VAL  299      15.435  64.087  23.350  1.00 40.94
ATOM   2278  O   VAL  299      14.321  64.612  23.461  1.00 41.66
ATOM   2279  N   LEU  300      16.337  64.091  24.328  1.00 41.41
ATOM   2280  CA  LEU  300      16.043  64.737  25.600  1.00 42.31
ATOM   2281  CB  LEU  300      16.973  64.224  26.713  1.00 41.48
ATOM   2282  CG  LEU  300      16.943  62.766  27.206  1.00 40.38
ATOM   2283  CD1 LEU  300      17.677  62.711  28.545  1.00 40.14
ATOM   2284  CD2 LEU  300      15.517  62.251  27.380  1.00 38.74
ATOM   2285  C   LEU  300      16.204  66.251  25.444  1.00 43.44
ATOM   2286  O   LEU  300      15.304  67.020  25.806  1.00 43.84
ATOM   2287  N   LEU  301      17.346  66.675  24.898  1.00 43.90
ATOM   2288  CA  LEU  301      17.603  68.100  24.707  1.00 43.85
ATOM   2289  CB  LEU  301      18.895  68.335  23.919  1.00 43.20
ATOM   2290  CG  LEU  301      20.211  67.969  24.613  1.00 43.48
ATOM   2291  CD1 LEU  301      21.385  68.372  23.730  1.00 43.37
ATOM   2292  CD2 LEU  301      20.307  68.675  25.955  1.00 43.71
ATOM   2293  C   LEU  301      16.444  68.738  23.969  1.00 44.11
ATOM   2294  O   LEU  301      16.068  69.875  24.254  1.00 44.38
ATOM   2295  N   ARG  302      15.863  68.007  23.025  1.00 44.45
ATOM   2296  CA  ARG  302      14.753  68.571  22.280  1.00 45.04
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Figure 4


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ATOM   2297  CB  ARG   302      14.296  67.660  21.148  1.00 45.49
ATOM   2298  CG  ARG   302      13.082  68.256  20.468  1.00 45.91
ATOM   2299  CD  ARG   302      12.391  67.327  19.514  1.00 46.45
ATOM   2300  NE  ARG   302      11.194  67.985  19.007  1.00 47.37
ATOM   2301  CZ  ARG   302      10.423  67.503  18.043  1.00 48.12
ATOM   2302  NH1 ARG   302      10.719  66.344  17.466  1.00 48.80
ATOM   2303  NH2 ARG   302       9.357  68.190  17.657  1.00 47.77
ATOM   2304  C   ARG   302      13.577  68.807  23.196  1.00 45.13
ATOM   2305  O   ARG   302      12.982  69.885  23.198  1.00 45.57
ATOM   2306  N   LEU   303      13.228  67.787  23.966  1.00 45.14
ATOM   2307  CA  LEU   303      12.113  67.918  24.883  1.00 45.18
ATOM   2308  CB  LEU   303      11.952  66.624  25.695  1.00 44.02
ATOM   2309  CG  LEU   303      11.495  65.427  24.846  1.00 42.43
ATOM   2310  CD1 LEU   303      11.365  64.162  25.690  1.00 41.06
ATOM   2311  CD2 LEU   303      10.154  65.784  24.207  1.00 41.96
ATOM   2312  C   LEU   303      12.359  69.133  25.783  1.00 45.83
ATOM   2313  O   LEU   303      11.444  69.919  26.044  1.00 45.85
ATOM   2314  N   VAL   304      13.599  69.302  26.232  1.00 46.44
ATOM   2315  CA  VAL   304      13.943  70.440  27.085  1.00 47.76
ATOM   2316  CB  VAL   304      15.443  70.426  27.496  1.00 47.79
ATOM   2317  CG1 VAL   304      15.866  71.815  27.996  1.00 46.89
ATOM   2318  CG2 VAL   304      15.678  69.386  28.581  1.00 47.81
ATOM   2319  C   VAL   304      13.666  71.764  26.371  1.00 48.44
ATOM   2320  O   VAL   304      12.899  72.596  26.861  1.00 48.95
ATOM   2321  N   ASP   305      14.297  71.946  25.212  1.00 48.52
ATOM   2322  CA  ASP   305      14.143  73.165  24.432  1.00 48.31
ATOM   2323  CB  ASP   305      14.968  73.067  23.143  1.00 49.45
ATOM   2324  CG  ASP   305      16.441  72.715  23.412  1.00 51.00
ATOM   2325  OD1 ASP   305      17.056  73.323  24.317  1.00 50.99
ATOM   2326  OD2 ASP   305      16.994  71.834  22.715  1.00 51.84
ATOM   2327  C   ASP   305      12.677  73.460  24.122  1.00 47.77
ATOM   2328  O   ASP   305      12.341  74.541  23.641  1.00 48.22
ATOM   2329  N   GLU   306      11.799  72.505  24.407  1.00 46.84
ATOM   2330  CA  GLU   306      10.378  72.713  24.176  1.00 46.34
ATOM   2331  CB  GLU   306       9.831  71.683  23.184  1.00 46.20
ATOM   2332  CG  GLU   306       9.866  72.216  21.761  1.00 48.15
ATOM   2333  CD  GLU   306       9.571  71.175  20.692  1.00 49.26
ATOM   2334  OE1 GLU   306       8.514  70.499  20.768  1.00 50.03
ATOM   2335  OE2 GLU   306      10.398  71.049  19.759  1.00 49.62
ATOM   2336  C   GLU   306       9.635  72.661  25.493  1.00 45.99
ATOM   2337  O   GLU   306       8.459  72.331  25.550  1.00 45.90
ATOM   2338  N   ASN   307      10.350  72.997  26.560  1.00 46.00
ATOM   2339  CA  ASN   307       9.787  73.029  27.902  1.00 45.60
ATOM   2340  CB  ASN   307       9.033  74.342  28.094  1.00 46.42
ATOM   2341  CG  ASN   307       9.971  75.531  28.224  1.00 46.98
ATOM   2342  OD1 ASN   307      10.435  75.849  29.321  1.00 47.63
ATOM   2343  ND2 ASN   307      10.273  76.181  27.102  1.00 46.93
ATOM   2344  C   ASN   307       8.886  71.853  28.246  1.00 45.05
ATOM   2345  O   ASN   307       7.812  72.029  28.829  1.00 45.19
ATOM   2346  N   LEU   308       9.336  70.650  27.900  1.00 44.24
ATOM   2347  CA  LEU   308       8.575  69.439  28.180  1.00 43.28
ATOM   2348  CB  LEU   308       8.376  68.637  26.893  1.00 43.27
ATOM   2349  CG  LEU   308       7.070  68.825  26.115  1.00 44.09
ATOM   2350  CD1 LEU   308       6.765  70.294  25.935  1.00 44.22
ATOM   2351  CD2 LEU   308       7.182  68.139  24.760  1.00 43.94
ATOM   2352  C   LEU   308       9.287  68.570  29.205  1.00 42.96
ATOM   2353  O   LEU   308       8.688  67.660  29.775  1.00 42.27
ATOM   2354  N   LEU   309      10.560  68.868  29.448  1.00 43.49
ATOM   2355  CA  LEU   309      11.368  68.077  30.371  1.00 44.85
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Figure 4

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ATOM   2356  CB  LEU  309      12.030  66.936  29.581  1.00 43.53
ATOM   2357  CG  LEU  309      12.958  65.925  30.254  1.00 42.07
ATOM   2358  CD1 LEU  309      12.235  65.226  31.390  1.00 40.83
ATOM   2359  CD2 LEU  309      13.416  64.913  29.212  1.00 42.11
ATOM   2360  C   LEU  309      12.436  68.900  31.108  1.00 46.21
ATOM   2361  O   LEU  309      13.074  69.777  30.518  1.00 46.04
ATOM   2362  N   PHE  310      12.625  68.601  32.397  1.00 47.92
ATOM   2363  CA  PHE  310      13.608  69.293  33.238  1.00 49.25
ATOM   2364  CB  PHE  310      15.013  69.093  32.666  1.00 48.20
ATOM   2365  CG  PHE  310      15.438  67.650  32.590  1.00 47.06
ATOM   2366  CD1 PHE  310      16.338  67.228  31.615  1.00 46.24
ATOM   2367  CD2 PHE  310      14.947  66.715  33.497  1.00 46.63
ATOM   2368  CE1 PHE  310      16.740  65.903  31.540  1.00 45.74
ATOM   2369  CE2 PHE  310      15.344  65.385  33.433  1.00 46.27
ATOM   2370  CZ  PHE  310      16.243  64.978  32.451  1.00 45.93
ATOM   2371  C   PHE  310      13.292  70.785  33.345  1.00 51.16
ATOM   2372  O   PHE  310      14.185  71.616  33.561  1.00 50.84
ATOM   2373  N   HIS  311      12.009  71.109  33.183  1.00 53.40
ATOM   2374  CA  HIS  311      11.529  72.482  33.262  1.00 55.80
ATOM   2375  CB  HIS  311      11.744  73.012  34.683  1.00 57.57
ATOM   2376  CG  HIS  311      11.212  72.098  35.745  1.00 59.78
ATOM   2377  CD2 HIS  311      11.848  71.363  36.689  1.00 60.29
ATOM   2378  ND1 HIS  311       9.867  71.815  35.879  1.00 60.36
ATOM   2379  CE1 HIS  311       9.699  70.944  36.860  1.00 60.99
ATOM   2380  NE2 HIS  311      10.885  70.654  37.368  1.00 60.85
ATOM   2381  C   HIS  311      12.214  73.384  32.236  1.00 56.24
ATOM   2382  O   HIS  311      12.288  74.608  32.415  1.00 56.87
ATOM   2383  N   GLY  312      12.705  72.772  31.159  1.00 55.96
ATOM   2384  CA  GLY  312      13.366  73.522  30.109  1.00 55.87
ATOM   2385  C   GLY  312      14.820  73.804  30.420  1.00 56.16
ATOM   2386  O   GLY  312      15.563  74.264  29.562  1.00 56.58
ATOM   2387  N   GLU  313      15.235  73.519  31.646  1.00 56.52
ATOM   2388  CA  GLU  313      16.612  73.765  32.048  1.00 57.69
ATOM   2389  CB  GLU  313      16.621  74.379  33.447  1.00 59.84
ATOM   2390  CG  GLU  313      15.849  75.698  33.515  1.00 63.16
ATOM   2391  CD  GLU  313      15.388  76.061  34.925  1.00 65.16
ATOM   2392  OE1 GLU  313      14.554  75.315  35.503  1.00 66.01
ATOM   2393  OE2 GLU  313      15.858  77.096  35.455  1.00 66.34
ATOM   2394  C   GLU  313      17.439  72.484  32.011  1.00 57.06
ATOM   2395  O   GLU  313      17.155  71.529  32.728  1.00 57.01
ATOM   2396  N   ALA  314      18.463  72.472  31.169  1.00 56.56
ATOM   2397  CA  ALA  314      19.316  71.305  31.029  1.00 56.76
ATOM   2398  CB  ALA  314      19.454  70.939  29.557  1.00 56.47
ATOM   2399  C   ALA  314      20.699  71.490  31.643  1.00 56.94
ATOM   2400  O   ALA  314      21.310  72.558  31.527  1.00 57.46
ATOM   2401  N   SER  315      21.183  70.422  32.276  1.00 56.73
ATOM   2402  CA  SER  315      22.487  70.383  32.932  1.00 56.15
ATOM   2403  CB  SER  315      22.666  69.029  33.624  1.00 56.44
ATOM   2404  OG  SER  315      23.981  68.868  34.130  1.00 57.39
ATOM   2405  C   SER  315      23.673  70.627  32.003  1.00 56.00
ATOM   2406  O   SER  315      23.595  70.416  30.793  1.00 55.42
ATOM   2407  N   GLU  316      24.776  71.070  32.598  1.00 56.67
ATOM   2408  CA  GLU  316      26.012  71.346  31.875  1.00 57.46
ATOM   2409  CB  GLU  316      27.111  71.754  32.860  1.00 58.71
ATOM   2410  CG  GLU  316      28.458  72.050  32.206  1.00 60.34
ATOM   2411  CD  GLU  316      28.442  73.343  31.406  1.00 61.64
ATOM   2412  OE1 GLU  316      28.288  74.420  32.031  1.00 62.41
ATOM   2413  OE2 GLU  316      28.574  73.280  30.160  1.00 61.76
ATOM   2414  C   GLU  316      26.442  70.078  31.161  1.00 57.35
```

Figure 4

ATOM	2415	O	GLU	316	26.770	70.088	29.972	1.00	57.68
ATOM	2416	N	GLN	317	26.439	68.988	31.920	1.00	56.84
ATOM	2417	CA	GLN	317	26.817	67.677	31.427	1.00	56.23
ATOM	2418	CB	GLN	317	26.760	66.669	32.580	1.00	55.93
ATOM	2419	CG	GLN	317	27.504	67.113	33.840	1.00	55.46
ATOM	2420	CD	GLN	317	27.063	66.355	35.085	1.00	55.01
ATOM	2421	OE1	GLN	317	27.246	65.140	35.194	1.00	54.83
ATOM	2422	NE2	GLN	317	26.468	67.074	36.029	1.00	54.68
ATOM	2423	C	GLN	317	25.902	67.210	30.290	1.00	56.37
ATOM	2424	O	GLN	317	26.376	66.634	29.312	1.00	56.16
ATOM	2425	N	LEU	318	24.599	67.476	30.412	1.00	56.41
ATOM	2426	CA	LEU	318	23.616	67.043	29.413	1.00	56.48
ATOM	2427	CB	LEU	318	22.190	67.333	29.890	1.00	55.59
ATOM	2428	CG	LEU	318	21.084	66.700	29.034	1.00	54.71
ATOM	2429	CD1	LEU	318	21.090	65.191	29.231	1.00	53.88
ATOM	2430	CD2	LEU	318	19.731	67.268	29.422	1.00	54.28
ATOM	2431	C	LEU	318	23.784	67.621	28.017	1.00	56.99
ATOM	2432	O	LEU	318	23.692	66.893	27.029	1.00	57.21
ATOM	2433	N	ARG	319	24.011	68.924	27.919	1.00	57.16
ATOM	2434	CA	ARG	319	24.177	69.530	26.606	1.00	57.68
ATOM	2435	CB	ARG	319	23.870	71.026	26.690	1.00	59.32
ATOM	2436	CG	ARG	319	22.420	71.284	27.105	1.00	62.20
ATOM	2437	CD	ARG	319	22.125	72.743	27.401	1.00	64.53
ATOM	2438	NE	ARG	319	20.758	72.927	27.892	1.00	66.89
ATOM	2439	CZ	ARG	319	20.297	74.055	28.433	1.00	68.29
ATOM	2440	NH1	ARG	319	21.096	75.112	28.555	1.00	68.30
ATOM	2441	NH2	ARG	319	19.034	74.127	28.851	1.00	68.25
ATOM	2442	C	ARG	319	25.587	69.278	26.081	1.00	57.09
ATOM	2443	O	ARG	319	26.049	69.951	25.160	1.00	57.05
ATOM	2444	N	THR	320	26.246	68.277	26.667	1.00	56.25
ATOM	2445	CA	THR	320	27.612	67.888	26.318	1.00	55.15
ATOM	2446	CB	THR	320	28.478	67.836	27.589	1.00	54.85
ATOM	2447	OG1	THR	320	28.601	69.158	28.133	1.00	54.94
ATOM	2448	CG2	THR	320	29.854	67.262	27.287	1.00	54.63
ATOM	2449	C	THR	320	27.689	66.524	25.613	1.00	55.04
ATOM	2450	O	THR	320	27.476	65.480	26.229	1.00	55.13
ATOM	2451	N	ARG	321	28.017	66.536	24.326	1.00	54.38
ATOM	2452	CA	ARG	321	28.106	65.304	23.545	1.00	54.36
ATOM	2453	CB	ARG	321	28.841	65.586	22.236	1.00	56.05
ATOM	2454	CG	ARG	321	28.153	66.651	21.402	1.00	59.03
ATOM	2455	CD	ARG	321	28.943	67.013	20.156	1.00	61.60
ATOM	2456	NE	ARG	321	28.331	68.123	19.426	1.00	63.68
ATOM	2457	CZ	ARG	321	28.909	68.753	18.406	1.00	65.43
ATOM	2458	NH1	ARG	321	30.119	68.381	17.997	1.00	65.83
ATOM	2459	NH2	ARG	321	28.280	69.750	17.792	1.00	65.76
ATOM	2460	C	ARG	321	28.765	64.123	24.262	1.00	52.97
ATOM	2461	O	ARG	321	29.885	64.234	24.758	1.00	53.13
ATOM	2462	N	GLY	322	28.056	62.996	24.316	1.00	51.39
ATOM	2463	CA	GLY	322	28.592	61.802	24.950	1.00	49.22
ATOM	2464	C	GLY	322	28.198	61.609	26.402	1.00	48.17
ATOM	2465	O	GLY	322	28.450	60.550	26.986	1.00	48.17
ATOM	2466	N	ALA	323	27.574	62.627	26.988	1.00	46.66
ATOM	2467	CA	ALA	323	27.150	62.573	28.385	1.00	44.99
ATOM	2468	CB	ALA	323	26.462	63.861	28.761	1.00	45.87
ATOM	2469	C	ALA	323	26.224	61.403	28.676	1.00	43.43
ATOM	2470	O	ALA	323	26.514	60.562	29.530	1.00	43.02
ATOM	2471	N	PHE	324	25.094	61.361	27.981	1.00	41.61
ATOM	2472	CA	PHE	324	24.147	60.282	28.185	1.00	40.44
ATOM	2473	CB	PHE	324	22.797	60.631	27.564	1.00	38.94

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ATOM   2474  CG  PHE  324      21.644  59.988  28.262  1.00 38.08
ATOM   2475  CD1 PHE  324      21.047  60.613  29.360  1.00 37.48
ATOM   2476  CD2 PHE  324      21.185  58.733  27.860  1.00 36.96
ATOM   2477  CE1 PHE  324      20.010  59.998  30.050  1.00 37.11
ATOM   2478  CE2 PHE  324      20.146  58.105  28.542  1.00 37.79
ATOM   2479  CZ  PHE  324      19.555  58.739  29.643  1.00 37.73
ATOM   2480  C   PHE  324      24.721  59.033  27.525  1.00 40.11
ATOM   2481  O   PHE  324      24.785  58.937  26.289  1.00 40.76
ATOM   2482  N   GLU  325      25.129  58.072  28.350  1.00 39.06
ATOM   2483  CA  GLU  325      25.740  56.851  27.844  1.00 37.85
ATOM   2484  CB  GLU  325      26.846  56.418  28.781  1.00 38.17
ATOM   2485  CG  GLU  325      27.790  57.528  29.085  1.00 40.68
ATOM   2486  CD  GLU  325      28.922  57.075  29.951  1.00 42.47
ATOM   2487  OE1 GLU  325      28.653  56.608  31.086  1.00 44.06
ATOM   2488  OE2 GLU  325      30.080  57.181  29.490  1.00 44.51
ATOM   2489  C   GLU  325      24.799  55.693  27.641  1.00 36.60
ATOM   2490  O   GLU  325      23.903  55.445  28.447  1.00 37.31
ATOM   2491  N   THR  326      25.019  54.968  26.554  1.00 35.30
ATOM   2492  CA  THR  326      24.193  53.816  26.245  1.00 33.37
ATOM   2493  CB  THR  326      24.875  52.921  25.207  1.00 31.58
ATOM   2494  OG1 THR  326      24.934  53.617  23.956  1.00 29.82
ATOM   2495  CG2 THR  326      24.113  51.619  25.041  1.00 29.94
ATOM   2496  C   THR  326      23.951  53.016  27.515  1.00 33.05
ATOM   2497  O   THR  326      22.846  52.528  27.742  1.00 33.99
ATOM   2498  N   ARG  327      24.981  52.902  28.349  1.00 32.29
ATOM   2499  CA  ARG  327      24.859  52.148  29.588  1.00 31.76
ATOM   2500  CB  ARG  327      26.146  52.245  30.417  1.00 33.30
ATOM   2501  CG  ARG  327      26.226  51.162  31.485  1.00 36.71
ATOM   2502  CD  ARG  327      27.596  51.043  32.177  1.00 38.88
ATOM   2503  NE  ARG  327      27.795  52.024  33.249  1.00 40.62
ATOM   2504  CZ  ARG  327      28.274  53.255  33.069  1.00 41.13
ATOM   2505  NH1 ARG  327      28.615  53.670  31.846  1.00 40.49
ATOM   2506  NH2 ARG  327      28.393  54.078  34.113  1.00 40.82
ATOM   2507  C   ARG  327      23.681  52.691  30.387  1.00 30.62
ATOM   2508  O   ARG  327      22.888  51.930  30.940  1.00 29.96
ATOM   2509  N   PHE  328      23.559  54.014  30.425  1.00 29.60
ATOM   2510  CA  PHE  328      22.479  54.660  31.154  1.00 28.70
ATOM   2511  CB  PHE  328      22.632  56.176  31.069  1.00 28.03
ATOM   2512  CG  PHE  328      23.903  56.684  31.686  1.00 27.73
ATOM   2513  CD1 PHE  328      24.337  57.975  31.439  1.00 27.37
ATOM   2514  CD2 PHE  328      24.678  55.857  32.505  1.00 28.92
ATOM   2515  CE1 PHE  328      25.526  58.437  31.992  1.00 28.75
ATOM   2516  CE2 PHE  328      25.871  56.305  33.069  1.00 28.74
ATOM   2517  CZ  PHE  328      26.298  57.599  32.812  1.00 28.68
ATOM   2518  C   PHE  328      21.135  54.226  30.590  1.00 29.06
ATOM   2519  O   PHE  328      20.189  53.953  31.351  1.00 29.59
ATOM   2520  N   VAL  329      21.057  54.154  29.257  1.00 28.40
ATOM   2521  CA  VAL  329      19.830  53.735  28.587  1.00 26.44
ATOM   2522  CB  VAL  329      20.040  53.552  27.059  1.00 25.14
ATOM   2523  CG1 VAL  329      18.737  53.107  26.387  1.00 22.55
ATOM   2524  CG2 VAL  329      20.542  54.841  26.444  1.00 23.05
ATOM   2525  C   VAL  329      19.388  52.399  29.166  1.00 27.98
ATOM   2526  O   VAL  329      18.240  52.239  29.576  1.00 27.88
ATOM   2527  N   SER  330      20.308  51.442  29.219  1.00 28.76
ATOM   2528  CA  SER  330      19.966  50.117  29.718  1.00 30.08
ATOM   2529  CB  SER  330      21.136  49.171  29.534  1.00 30.45
ATOM   2530  OG  SER  330      20.720  47.852  29.822  1.00 31.92
ATOM   2531  C   SER  330      19.534  50.107  31.172  1.00 31.40
ATOM   2532  O   SER  330      18.690  49.298  31.577  1.00 31.74
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Figure 4

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ATOM   2533  N   GLN   331      20.118  50.993  31.972  1.00 32.45
ATOM   2534  CA  GLN   331      19.745  51.061  33.381  1.00 33.16
ATOM   2535  CB  GLN   331      20.668  51.992  34.151  1.00 33.58
ATOM   2536  CG  GLN   331      22.093  51.540  34.194  1.00 35.83
ATOM   2537  CD  GLN   331      22.947  52.534  34.919  1.00 37.72
ATOM   2538  OE1 GLN   331      22.626  52.927  36.043  1.00 39.62
ATOM   2539  NE2 GLN   331      24.042  52.958  34.291  1.00 38.98
ATOM   2540  C   GLN   331      18.327  51.591  33.482  1.00 33.78
ATOM   2541  O   GLN   331      17.428  50.881  33.938  1.00 34.06
ATOM   2542  N   VAL   332      18.129  52.835  33.038  1.00 33.77
ATOM   2543  CA  VAL   332      16.808  53.457  33.097  1.00 33.65
ATOM   2544  CB  VAL   332      16.760  54.791  32.282  1.00 32.19
ATOM   2545  CG1 VAL   332      17.279  54.584  30.905  1.00 33.04
ATOM   2546  CG2 VAL   332      15.340  55.312  32.215  1.00 31.67
ATOM   2547  C   VAL   332      15.695  52.505  32.638  1.00 34.20
ATOM   2548  O   VAL   332      14.571  52.566  33.139  1.00 34.51
ATOM   2549  N   GLU   333      16.001  51.607  31.711  1.00 34.30
ATOM   2550  CA  GLU   333      14.981  50.676  31.258  1.00 34.92
ATOM   2551  CB  GLU   333      15.210  50.289  29.795  1.00 34.40
ATOM   2552  CG  GLU   333      14.893  51.413  28.837  1.00 33.07
ATOM   2553  CD  GLU   333      14.806  50.956  27.409  1.00 31.80
ATOM   2554  OE1 GLU   333      13.983  50.060  27.114  1.00 31.65
ATOM   2555  OE2 GLU   333      15.561  51.504  26.581  1.00 31.72
ATOM   2556  C   GLU   333      14.949  49.438  32.135  1.00 35.76
ATOM   2557  O   GLU   333      14.163  48.520  31.911  1.00 35.73
ATOM   2558  N   SER   334      15.814  49.419  33.138  1.00 36.91
ATOM   2559  CA  SER   334      15.876  48.307  34.071  1.00 38.13
ATOM   2560  CB  SER   334      17.328  47.934  34.346  1.00 39.38
ATOM   2561  OG  SER   334      17.460  46.524  34.468  1.00 41.52
ATOM   2562  C   SER   334      15.201  48.747  35.362  1.00 37.93
ATOM   2563  O   SER   334      15.053  47.973  36.306  1.00 38.63
ATOM   2564  N   ASP   335      14.807  50.014  35.385  1.00 38.51
ATOM   2565  CA  ASP   335      14.133  50.619  36.521  1.00 38.59
ATOM   2566  CB  ASP   335      13.776  52.061  36.173  1.00 39.10
ATOM   2567  CG  ASP   335      13.346  52.864  37.373  1.00 39.89
ATOM   2568  OD1 ASP   335      12.278  52.547  37.950  1.00 40.30
ATOM   2569  OD2 ASP   335      14.079  53.816  37.737  1.00 39.90
ATOM   2570  C   ASP   335      12.876  49.809  36.840  1.00 39.11
ATOM   2571  O   ASP   335      12.241  49.249  35.945  1.00 39.03
ATOM   2572  N   THR   336      12.517  49.768  38.119  1.00 39.68
ATOM   2573  CA  THR   336      11.372  48.999  38.605  1.00 39.94
ATOM   2574  CB  THR   336      11.773  48.297  39.896  1.00 39.68
ATOM   2575  OG1 THR   336      12.901  47.464  39.630  1.00 40.95
ATOM   2576  CG2 THR   336      10.650  47.452  40.426  1.00 39.84
ATOM   2577  C   THR   336      10.043  49.735  38.853  1.00 40.52
ATOM   2578  O   THR   336       8.984  49.108  38.931  1.00 40.91
ATOM   2579  N   GLY   337      10.085  51.054  38.970  1.00 40.80
ATOM   2580  CA  GLY   337       8.870  51.804  39.234  1.00 41.83
ATOM   2581  C   GLY   337       9.307  52.948  40.112  1.00 42.60
ATOM   2582  O   GLY   337       8.990  54.105  39.865  1.00 43.33
ATOM   2583  N   ASP   338      10.043  52.604  41.156  1.00 43.47
ATOM   2584  CA  ASP   338      10.606  53.589  42.059  1.00 44.40
ATOM   2585  CB  ASP   338      11.354  52.868  43.175  1.00 44.83
ATOM   2586  CG  ASP   338      12.303  51.808  42.637  1.00 45.34
ATOM   2587  OD1 ASP   338      11.879  51.032  41.751  1.00 46.12
ATOM   2588  OD2 ASP   338      13.465  51.742  43.087  1.00 45.59
ATOM   2589  C   ASP   338      11.597  54.296  41.142  1.00 44.84
ATOM   2590  O   ASP   338      12.605  53.709  40.756  1.00 45.53
ATOM   2591  N   ARG   339      11.310  55.533  40.763  1.00 44.81
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Figure 4

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ATOM   2592  CA  ARG  339      12.208  56.256  39.874  1.00 45.11
ATOM   2593  CB  ARG  339      11.702  57.687  39.654  1.00 45.72
ATOM   2594  CG  ARG  339      10.466  57.799  38.783  1.00 46.11
ATOM   2595  CD  ARG  339       9.201  57.413  39.521  1.00 46.99
ATOM   2596  NE  ARG  339       8.041  57.492  38.633  1.00 47.58
ATOM   2597  CZ  ARG  339       6.780  57.326  39.017  1.00 47.30
ATOM   2598  NH1 ARG  339       6.492  57.068  40.287  1.00 47.38
ATOM   2599  NH2 ARG  339       5.806  57.413  38.123  1.00 47.44
ATOM   2600  C   ARG  339      13.637  56.295  40.419  1.00 44.98
ATOM   2601  O   ARG  339      14.466  57.084  39.960  1.00 44.83
ATOM   2602  N   LYS  340      13.922  55.441  41.394  1.00 44.75
ATOM   2603  CA  LYS  340      15.238  55.394  42.001  1.00 45.05
ATOM   2604  CB  LYS  340      15.341  54.179  42.917  1.00 46.19
ATOM   2605  CG  LYS  340      14.358  54.250  44.081  1.00 47.87
ATOM   2606  CD  LYS  340      14.598  53.154  45.094  1.00 49.25
ATOM   2607  CE  LYS  340      13.365  52.949  45.957  1.00 50.44
ATOM   2608  NZ  LYS  340      13.353  51.589  46.598  1.00 51.78
ATOM   2609  C   LYS  340      16.398  55.422  41.014  1.00 44.66
ATOM   2610  O   LYS  340      17.186  56.372  41.026  1.00 44.90
ATOM   2611  N   GLN  341      16.509  54.408  40.155  1.00 43.94
ATOM   2612  CA  GLN  341      17.603  54.362  39.174  1.00 42.93
ATOM   2613  CB  GLN  341      17.598  53.028  38.435  1.00 45.04
ATOM   2614  CG  GLN  341      18.035  51.860  39.289  1.00 48.03
ATOM   2615  CD  GLN  341      18.758  50.801  38.482  1.00 49.69
ATOM   2616  OE1 GLN  341      19.731  51.101  37.779  1.00 50.67
ATOM   2617  NE2 GLN  341      18.297  49.556  38.581  1.00 50.43
ATOM   2618  C   GLN  341      17.616  55.497  38.146  1.00 40.93
ATOM   2619  O   GLN  341      18.672  56.057  37.839  1.00 38.85
ATOM   2620  N   ILE  342      16.449  55.824  37.600  1.00 39.61
ATOM   2621  CA  ILE  342      16.364  56.905  36.624  1.00 39.07
ATOM   2622  CB  ILE  342      14.920  57.110  36.130  1.00 39.24
ATOM   2623  CG2 ILE  342      14.880  58.226  35.107  1.00 39.19
ATOM   2624  CG1 ILE  342      14.392  55.817  35.501  1.00 39.87
ATOM   2625  CD1 ILE  342      12.945  55.902  35.070  1.00 40.76
ATOM   2626  C   ILE  342      16.832  58.185  37.301  1.00 38.43
ATOM   2627  O   ILE  342      17.704  58.892  36.795  1.00 37.48
ATOM   2628  N   TYR  343      16.240  58.466  38.456  1.00 38.93
ATOM   2629  CA  TYR  343      16.580  59.647  39.236  1.00 39.71
ATOM   2630  CB  TYR  343      15.813  59.656  40.567  1.00 40.97
ATOM   2631  CG  TYR  343      16.173  60.835  41.448  1.00 42.53
ATOM   2632  CD1 TYR  343      15.344  61.954  41.521  1.00 43.30
ATOM   2633  CE1 TYR  343      15.730  63.092  42.228  1.00 44.58
ATOM   2634  CD2 TYR  343      17.397  60.880  42.119  1.00 43.04
ATOM   2635  CE2 TYR  343      17.791  62.014  42.826  1.00 43.55
ATOM   2636  CZ  TYR  343      16.958  63.117  42.872  1.00 44.31
ATOM   2637  OH  TYR  343      17.369  64.260  43.523  1.00 45.74
ATOM   2638  C   TYR  343      18.070  59.635  39.532  1.00 39.93
ATOM   2639  O   TYR  343      18.789  60.598  39.262  1.00 40.28
ATOM   2640  N   ASN  344      18.525  58.529  40.098  1.00 40.14
ATOM   2641  CA  ASN  344      19.924  58.371  40.460  1.00 40.97
ATOM   2642  CB  ASN  344      20.146  56.958  40.989  1.00 42.94
ATOM   2643  CG  ASN  344      21.287  56.880  41.977  1.00 44.68
ATOM   2644  OD1 ASN  344      22.448  57.137  41.628  1.00 46.05
ATOM   2645  ND2 ASN  344      20.965  56.531  43.225  1.00 44.93
ATOM   2646  C   ASN  344      20.869  58.649  39.292  1.00 40.46
ATOM   2647  O   ASN  344      21.946  59.208  39.483  1.00 40.33
ATOM   2648  N   ILE  345      20.460  58.262  38.085  1.00 40.50
ATOM   2649  CA  ILE  345      21.280  58.467  36.890  1.00 39.89
ATOM   2650  CB  ILE  345      20.803  57.555  35.720  1.00 39.76
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ATOM   2651  CG2 ILE   345      21.597  57.849  34.448  1.00 38.62
ATOM   2652  CG1 ILE   345      20.966  56.090  36.114  1.00 38.74
ATOM   2653  CD1 ILE   345      20.201  55.151  35.242  1.00 38.61
ATOM   2654  C   ILE   345      21.247  59.924  36.434  1.00 39.80
ATOM   2655  O   ILE   345      22.281  60.490  36.074  1.00 39.67
ATOM   2656  N   LEU   346      20.062  60.529  36.449  1.00 39.59
ATOM   2657  CA  LEU   346      19.912  61.923  36.029  1.00 39.58
ATOM   2658  CB  LEU   346      18.434  62.255  35.818  1.00 37.79
ATOM   2659  CG  LEU   346      17.809  61.528  34.625  1.00 36.58
ATOM   2660  CD1 LEU   346      16.277  61.599  34.684  1.00 35.18
ATOM   2661  CD2 LEU   346      18.363  62.145  33.337  1.00 35.05
ATOM   2662  C   LEU   346      20.519  62.892  37.034  1.00 40.82
ATOM   2663  O   LEU   346      21.177  63.857  36.654  1.00 41.02
ATOM   2664  N   SER   347      20.298  62.646  38.322  1.00 42.34
ATOM   2665  CA  SER   347      20.859  63.530  39.339  1.00 43.44
ATOM   2666  CB  SER   347      20.491  63.042  40.745  1.00 43.90
ATOM   2667  OG  SER   347      20.665  61.639  40.868  1.00 45.32
ATOM   2668  C   SER   347      22.368  63.556  39.156  1.00 43.44
ATOM   2669  O   SER   347      22.974  64.624  39.051  1.00 44.11
ATOM   2670  N   THR   348      22.969  62.374  39.096  1.00 43.10
ATOM   2671  CA  THR   348      24.407  62.285  38.909  1.00 42.97
ATOM   2672  CB  THR   348      24.853  60.830  38.700  1.00 42.31
ATOM   2673  OG1 THR   348      24.666  60.096  39.918  1.00 42.08
ATOM   2674  CG2 THR   348      26.322  60.780  38.282  1.00 40.85
ATOM   2675  C   THR   348      24.798  63.093  37.683  1.00 43.25
ATOM   2676  O   THR   348      25.796  63.813  37.680  1.00 43.52
ATOM   2677  N   LEU   349      23.990  62.982  36.640  1.00 43.57
ATOM   2678  CA  LEU   349      24.271  63.697  35.412  1.00 44.17
ATOM   2679  CB  LEU   349      23.343  63.180  34.311  1.00 44.43
ATOM   2680  CG  LEU   349      23.787  63.204  32.847  1.00 44.86
ATOM   2681  CD1 LEU   349      25.198  62.658  32.688  1.00 44.59
ATOM   2682  CD2 LEU   349      22.790  62.375  32.046  1.00 44.64
ATOM   2683  C   LEU   349      24.102  65.201  35.638  1.00 44.32
ATOM   2684  O   LEU   349      24.317  66.003  34.726  1.00 45.33
ATOM   2685  N   GLY   350      23.722  65.574  36.862  1.00 43.94
ATOM   2686  CA  GLY   350      23.559  66.981  37.210  1.00 43.15
ATOM   2687  C   GLY   350      22.167  67.570  37.038  1.00 42.49
ATOM   2688  O   GLY   350      22.024  68.752  36.703  1.00 41.70
ATOM   2689  N   LEU   351      21.143  66.758  37.288  1.00 41.97
ATOM   2690  CA  LEU   351      19.758  67.197  37.132  1.00 41.45
ATOM   2691  CB  LEU   351      19.194  66.676  35.812  1.00 40.99
ATOM   2692  CG  LEU   351      19.875  67.115  34.522  1.00 40.66
ATOM   2693  CD1 LEU   351      19.516  66.144  33.416  1.00 41.63
ATOM   2694  CD2 LEU   351      19.453  68.533  34.172  1.00 40.77
ATOM   2695  C   LEU   351      18.858  66.718  38.262  1.00 41.15
ATOM   2696  O   LEU   351      19.170  65.760  38.973  1.00 40.88
ATOM   2697  N   ARG   352      17.720  67.379  38.410  1.00 41.10
ATOM   2698  CA  ARG   352      16.782  67.007  39.457  1.00 41.25
ATOM   2699  CB  ARG   352      16.614  68.173  40.431  1.00 42.65
ATOM   2700  CG  ARG   352      17.929  68.581  41.070  1.00 43.68
ATOM   2701  CD  ARG   352      18.504  67.421  41.851  1.00 45.59
ATOM   2702  NE  ARG   352      19.960  67.478  41.917  1.00 47.73
ATOM   2703  CZ  ARG   352      20.715  66.567  42.521  1.00 48.77
ATOM   2704  NH1 ARG   352      20.143  65.524  43.119  1.00 49.05
ATOM   2705  NH2 ARG   352      22.038  66.700  42.519  1.00 49.14
ATOM   2706  C   ARG   352      15.458  66.621  38.827  1.00 39.59
ATOM   2707  O   ARG   352      14.512  67.399  38.793  1.00 40.34
ATOM   2708  N   PRO   353      15.378  65.388  38.324  1.00 38.06
ATOM   2709  CD  PRO   353      16.325  64.285  38.555  1.00 37.28
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Figure 4

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ATOM   2710  CA  PRO  353      14.159  64.901  37.683  1.00 37.45
ATOM   2711  CB  PRO  353      14.595  63.552  37.134  1.00 37.27
ATOM   2712  CG  PRO  353      15.491  63.064  38.232  1.00 36.92
ATOM   2713  C   PRO  353      12.998  64.763  38.650  1.00 36.35
ATOM   2714  O   PRO  353      13.180  64.360  39.791  1.00 36.28
ATOM   2715  N   SER  354      11.805  65.110  38.194  1.00 35.82
ATOM   2716  CA  SER  354      10.625  64.951  39.028  1.00 36.40
ATOM   2717  CB  SER  354       9.570  66.010  38.698  1.00 35.94
ATOM   2718  OG  SER  354       8.944  65.725  37.459  1.00 35.63
ATOM   2719  C   SER  354      10.091  63.570  38.653  1.00 36.41
ATOM   2720  O   SER  354      10.592  62.948  37.716  1.00 37.42
ATOM   2721  N   THR  355       9.087  63.091  39.375  1.00 36.02
ATOM   2722  CA  THR  355       8.493  61.790  39.099  1.00 35.68
ATOM   2723  CB  THR  355       7.200  61.615  39.923  1.00 36.38
ATOM   2724  OG1 THR  355       7.525  61.645  41.316  1.00 37.75
ATOM   2725  CG2 THR  355       6.510  60.293  39.598  1.00 36.44
ATOM   2726  C   THR  355       8.161  61.633  37.609  1.00 35.80
ATOM   2727  O   THR  355       8.319  60.548  37.029  1.00 34.73
ATOM   2728  N   THR  356       7.698  62.720  36.994  1.00 35.28
ATOM   2729  CA  THR  356       7.336  62.690  35.586  1.00 35.39
ATOM   2730  CB  THR  356       6.287  63.774  35.263  1.00 35.59
ATOM   2731  OG1 THR  356       6.651  64.990  35.925  1.00 35.39
ATOM   2732  CG2 THR  356       4.892  63.331  35.719  1.00 34.33
ATOM   2733  C   THR  356       8.542  62.848  34.662  1.00 35.30
ATOM   2734  O   THR  356       8.560  62.285  33.559  1.00 34.91
ATOM   2735  N   ASP  357       9.537  63.624  35.089  1.00 35.07
ATOM   2736  CA  ASP  357      10.740  63.782  34.277  1.00 35.80
ATOM   2737  CB  ASP  357      11.804  64.598  35.012  1.00 36.76
ATOM   2738  CG  ASP  357      11.451  66.077  35.116  1.00 38.19
ATOM   2739  OD1 ASP  357      11.475  66.778  34.071  1.00 37.60
ATOM   2740  OD2 ASP  357      11.158  66.538  36.249  1.00 38.76
ATOM   2741  C   ASP  357      11.277  62.373  34.039  1.00 35.97
ATOM   2742  O   ASP  357      11.460  61.942  32.901  1.00 36.94
ATOM   2743  N   CYS  358      11.498  61.649  35.131  1.00 35.67
ATOM   2744  CA  CYS  358      12.013  60.293  35.057  1.00 35.44
ATOM   2745  CB  CYS  358      12.051  59.658  36.447  1.00 35.93
ATOM   2746  SG  CYS  358      13.247  60.410  37.575  1.00 35.81
ATOM   2747  C   CYS  358      11.177  59.433  34.138  1.00 34.88
ATOM   2748  O   CYS  358      11.711  58.698  33.308  1.00 35.87
ATOM   2749  N   ASP  359       9.863  59.517  34.290  1.00 34.10
ATOM   2750  CA  ASP  359       8.960  58.729  33.464  1.00 33.10
ATOM   2751  CB  ASP  359       7.519  58.964  33.910  1.00 35.03
ATOM   2752  CG  ASP  359       7.118  58.058  35.062  1.00 36.65
ATOM   2753  OD1 ASP  359       7.950  57.850  35.975  1.00 38.15
ATOM   2754  OD2 ASP  359       5.969  57.561  35.055  1.00 37.12
ATOM   2755  C   ASP  359       9.130  59.058  31.985  1.00 31.16
ATOM   2756  O   ASP  359       9.090  58.170  31.133  1.00 30.01
ATOM   2757  N   ILE  360       9.325  60.334  31.682  1.00 29.54
ATOM   2758  CA  ILE  360       9.524  60.741  30.300  1.00 28.61
ATOM   2759  CB  ILE  360       9.546  62.273  30.162  1.00 27.75
ATOM   2760  CG2 ILE  360      10.255  62.668  28.874  1.00 27.01
ATOM   2761  CG1 ILE  360       8.112  62.818  30.235  1.00 26.18
ATOM   2762  CD1 ILE  360       8.024  64.322  30.190  1.00 23.23
ATOM   2763  C   ILE  360      10.857  60.176  29.825  1.00 29.21
ATOM   2764  O   ILE  360      10.919  59.480  28.805  1.00 29.88
ATOM   2765  N   VAL  361      11.923  60.466  30.569  1.00 28.39
ATOM   2766  CA  VAL  361      13.248  59.971  30.219  1.00 28.01
ATOM   2767  CB  VAL  361      14.258  60.256  31.342  1.00 27.73
ATOM   2768  CG1 VAL  361      15.575  59.551  31.055  1.00 27.43
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Figure 4

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ATOM   2769  CG2 VAL   361      14.492  61.759  31.453  1.00 27.76
ATOM   2770  C   VAL   361      13.245  58.464  29.919  1.00 27.74
ATOM   2771  O   VAL   361      14.055  57.982  29.107  1.00 27.40
ATOM   2772  N   ARG   362      12.341  57.719  30.556  1.00 27.72
ATOM   2773  CA  ARG   362      12.277  56.275  30.325  1.00 27.95
ATOM   2774  CB  ARG   362      11.523  55.571  31.455  1.00 29.48
ATOM   2775  CG  ARG   362      11.137  54.147  31.101  1.00 31.97
ATOM   2776  CD  ARG   362      10.900  53.266  32.308  1.00 33.93
ATOM   2777  NE  ARG   362      10.930  51.859  31.893  1.00 37.37
ATOM   2778  CZ  ARG   362      10.938  50.817  32.725  1.00 37.52
ATOM   2779  NH1 ARG   362      10.920  51.010  34.043  1.00 38.72
ATOM   2780  NH2 ARG   362      10.960  49.582  32.230  1.00 36.06
ATOM   2781  C   ARG   362      11.614  55.959  28.994  1.00 27.88
ATOM   2782  O   ARG   362      12.016  55.032  28.289  1.00 29.02
ATOM   2783  N   ARG   363      10.586  56.728  28.660  1.00 27.31
ATOM   2784  CA  ARG   363       9.866  56.564  27.400  1.00 25.77
ATOM   2785  CB  ARG   363       8.641  57.486  27.374  1.00 26.51
ATOM   2786  CG  ARG   363       7.530  57.084  28.318  1.00 26.30
ATOM   2787  CD  ARG   363       6.730  55.929  27.739  1.00 28.36
ATOM   2788  NE  ARG   363       6.259  56.216  26.380  1.00 30.91
ATOM   2789  CZ  ARG   363       6.872  55.826  25.260  1.00 31.55
ATOM   2790  NH1 ARG   363       7.992  55.112  25.315  1.00 33.18
ATOM   2791  NH2 ARG   363       6.370  56.158  24.077  1.00 32.30
ATOM   2792  C   ARG   363      10.817  56.949  26.272  1.00 24.71
ATOM   2793  O   ARG   363      10.748  56.392  25.175  1.00 24.40
ATOM   2794  N   ALA   364      11.706  57.905  26.540  1.00 23.90
ATOM   2795  CA  ALA   364      12.653  58.339  25.507  1.00 24.48
ATOM   2796  CB  ALA   364      13.463  59.545  25.969  1.00 23.15
ATOM   2797  C   ALA   364      13.571  57.176  25.226  1.00 25.01
ATOM   2798  O   ALA   364      13.854  56.872  24.069  1.00 26.22
ATOM   2799  N   CYS   365      14.023  56.518  26.290  1.00 25.03
ATOM   2800  CA  CYS   365      14.902  55.370  26.157  1.00 24.77
ATOM   2801  CB  CYS   365      15.450  54.970  27.528  1.00 23.03
ATOM   2802  SG  CYS   365      16.728  56.114  28.173  1.00 21.60
ATOM   2803  C   CYS   365      14.140  54.206  25.514  1.00 26.44
ATOM   2804  O   CYS   365      14.661  53.535  24.617  1.00 27.49
ATOM   2805  N   GLU   366      12.906  53.956  25.944  1.00 26.87
ATOM   2806  CA  GLU   366      12.145  52.859  25.342  1.00 27.98
ATOM   2807  CB  GLU   366      10.757  52.743  25.988  1.00 28.74
ATOM   2808  CG  GLU   366      10.785  52.431  27.490  1.00 30.75
ATOM   2809  CD  GLU   366       9.427  51.981  28.041  1.00 32.09
ATOM   2810  OE1 GLU   366       8.444  52.757  27.970  1.00 32.39
ATOM   2811  OE2 GLU   366       9.342  50.841  28.547  1.00 33.30
ATOM   2812  C   GLU   366      12.005  53.056  23.815  1.00 28.15
ATOM   2813  O   GLU   366      12.117  52.104  23.029  1.00 27.63
ATOM   2814  N   SER   367      11.776  54.304  23.407  1.00 28.42
ATOM   2815  CA  SER   367      11.612  54.650  21.993  1.00 27.23
ATOM   2816  CB  SER   367      11.368  56.156  21.833  1.00 27.45
ATOM   2817  OG  SER   367      10.161  56.552  22.447  1.00 27.44
ATOM   2818  C   SER   367      12.824  54.276  21.165  1.00 26.52
ATOM   2819  O   SER   367      12.724  53.567  20.162  1.00 27.99
ATOM   2820  N   VAL   368      13.977  54.773  21.581  1.00 24.30
ATOM   2821  CA  VAL   368      15.194  54.499  20.849  1.00 22.45
ATOM   2822  CB  VAL   368      16.324  55.395  21.375  1.00 20.96
ATOM   2823  CG1 VAL   368      17.623  55.075  20.682  1.00 18.44
ATOM   2824  CG2 VAL   368      15.928  56.843  21.190  1.00 18.99
ATOM   2825  C   VAL   368      15.605  53.019  20.888  1.00 23.13
ATOM   2826  O   VAL   368      15.850  52.420  19.832  1.00 23.88
ATOM   2827  N   SER   369      15.660  52.405  22.071  1.00 22.54
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Figure 4

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ATOM   2828  CA  SER  369      16.071  51.003  22.106  1.00 21.93
ATOM   2829  CB  SER  369      16.248  50.476  23.542  1.00 23.39
ATOM   2830  OG  SER  369      15.011  50.251  24.197  1.00 25.91
ATOM   2831  C   SER  369      15.109  50.112  21.348  1.00 20.54
ATOM   2832  O   SER  369      15.526  49.063  20.850  1.00 20.31
ATOM   2833  N   THR  370      13.832  50.499  21.259  1.00 18.40
ATOM   2834  CA  THR  370      12.878  49.682  20.496  1.00 17.32
ATOM   2835  CB  THR  370      11.400  49.976  20.859  1.00 16.46
ATOM   2836  OG1 THR  370      11.053  49.298  22.073  1.00 15.81
ATOM   2837  CG2 THR  370      10.473  49.487  19.774  1.00 14.39
ATOM   2838  C   THR  370      13.076  49.936  19.001  1.00 17.03
ATOM   2839  O   THR  370      12.977  49.008  18.186  1.00 17.38
ATOM   2840  N   ARG  371      13.358  51.177  18.617  1.00 16.71
ATOM   2841  CA  ARG  371      13.562  51.423  17.201  1.00 16.54
ATOM   2842  CB  ARG  371      13.810  52.905  16.882  1.00 17.42
ATOM   2843  CG  ARG  371      14.013  53.123  15.374  1.00 17.76
ATOM   2844  CD  ARG  371      14.283  54.559  14.943  1.00 17.40
ATOM   2845  NE  ARG  371      15.567  55.076  15.412  1.00 18.85
ATOM   2846  CZ  ARG  371      16.159  56.154  14.896  1.00 18.99
ATOM   2847  NH1 ARG  371      15.583  56.810  13.892  1.00 17.43
ATOM   2848  NH2 ARG  371      17.303  56.605  15.406  1.00 19.19
ATOM   2849  C   ARG  371      14.763  50.607  16.759  1.00 15.91
ATOM   2850  O   ARG  371      14.689  49.929  15.748  1.00 17.14
ATOM   2851  N   ALA  372      15.856  50.644  17.519  1.00 15.40
ATOM   2852  CA  ALA  372      17.061  49.883  17.148  1.00 16.23
ATOM   2853  CB  ALA  372      18.152  50.046  18.197  1.00 15.66
ATOM   2854  C   ALA  372      16.775  48.407  16.957  1.00 16.83
ATOM   2855  O   ALA  372      17.125  47.838  15.923  1.00 18.06
ATOM   2856  N   ALA  373      16.149  47.790  17.955  1.00 16.86
ATOM   2857  CA  ALA  373      15.817  46.367  17.912  1.00 17.10
ATOM   2858  CB  ALA  373      15.027  45.976  19.156  1.00 16.66
ATOM   2859  C   ALA  373      15.024  46.018  16.665  1.00 18.79
ATOM   2860  O   ALA  373      15.301  45.004  16.018  1.00 20.02
ATOM   2861  N   HIS  374      14.037  46.841  16.316  1.00 19.22
ATOM   2862  CA  HIS  374      13.243  46.560  15.122  1.00 20.89
ATOM   2863  CB  HIS  374      12.025  47.489  15.052  1.00 20.98
ATOM   2864  CG  HIS  374      10.948  47.131  16.029  1.00 19.79
ATOM   2865  CD2 HIS  374      10.813  46.065  16.855  1.00 19.53
ATOM   2866  ND1 HIS  374       9.833  47.914  16.229  1.00 19.92
ATOM   2867  CE1 HIS  374       9.057  47.347  17.137  1.00 18.78
ATOM   2868  NE2 HIS  374       9.629  46.223  17.532  1.00 18.61
ATOM   2869  C   HIS  374      14.075  46.696  13.866  1.00 21.57
ATOM   2870  O   HIS  374      14.136  45.789  13.058  1.00 21.42
ATOM   2871  N   MSE  375      14.722  47.835  13.698  1.00 24.00
ATOM   2872  CA  MSE  375      15.561  48.027  12.528  1.00 26.05
ATOM   2873  CB  MSE  375      16.390  49.311  12.666  1.00 28.31
ATOM   2874  CG  MSE  375      15.671  50.558  12.197  1.00 31.46
ATOM   2875  SE  MSE  375      15.246  50.448  10.400  1.00 41.26
ATOM   2876  CE  MSE  375      16.340  51.745   9.680  1.00 36.51
ATOM   2877  C   MSE  375      16.476  46.810  12.390  1.00 25.84
ATOM   2878  O   MSE  375      16.501  46.159  11.351  1.00 26.84
ATOM   2879  N   CYS  376      17.200  46.489  13.455  1.00 25.61
ATOM   2880  CA  CYS  376      18.107  45.349  13.436  1.00 25.11
ATOM   2881  CB  CYS  376      18.693  45.117  14.831  1.00 26.04
ATOM   2882  SG  CYS  376      20.038  43.879  14.876  1.00 27.98
ATOM   2883  C   CYS  376      17.445  44.058  12.931  1.00 24.01
ATOM   2884  O   CYS  376      18.015  43.369  12.078  1.00 24.35
ATOM   2885  N   SER  377      16.251  43.741  13.443  1.00 22.14
ATOM   2886  CA  SER  377      15.519  42.531  13.038  1.00 20.58
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Figure 4

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ATOM   2887  CB  SER   377      14.203  42.399  13.811  1.00 20.36
ATOM   2888  OG  SER   377      13.233  43.325  13.338  1.00 20.95
ATOM   2889  C   SER   377      15.210  42.535  11.542  1.00 20.00
ATOM   2890  O   SER   377      15.154  41.484  10.900  1.00 19.23
ATOM   2891  N   ALA   378      14.995  43.715  10.980  1.00 19.64
ATOM   2892  CA  ALA   378      14.723  43.787   9.549  1.00 19.32
ATOM   2893  CB  ALA   378      14.521  45.243   9.119  1.00 18.02
ATOM   2894  C   ALA   378      15.958  43.186   8.874  1.00 19.40
ATOM   2895  O   ALA   378      15.860  42.230   8.093  1.00 18.55
ATOM   2896  N   GLY   379      17.123  43.740   9.222  1.00 20.18
ATOM   2897  CA  GLY   379      18.381  43.271   8.669  1.00 20.06
ATOM   2898  C   GLY   379      18.547  41.762   8.734  1.00 19.52
ATOM   2899  O   GLY   379      18.754  41.113   7.704  1.00 20.07
ATOM   2900  N   LEU   380      18.442  41.201   9.936  1.00 18.61
ATOM   2901  CA  LEU   380      18.596  39.763  10.110  1.00 18.74
ATOM   2902  CB  LEU   380      18.489  39.371  11.579  1.00 18.49
ATOM   2903  CG  LEU   380      18.774  37.881  11.816  1.00 17.82
ATOM   2904  CD1 LEU   380      20.215  37.586  11.383  1.00 16.94
ATOM   2905  CD2 LEU   380      18.557  37.512  13.285  1.00 16.34
ATOM   2906  C   LEU   380      17.580  38.938   9.341  1.00 19.56
ATOM   2907  O   LEU   380      17.895  37.833   8.892  1.00 20.67
ATOM   2908  N   ALA   381      16.354  39.447   9.211  1.00 19.83
ATOM   2909  CA  ALA   381      15.311  38.713   8.496  1.00 20.17
ATOM   2910  CB  ALA   381      13.961  39.327   8.759  1.00 19.87
ATOM   2911  C   ALA   381      15.638  38.746   7.009  1.00 21.06
ATOM   2912  O   ALA   381      15.421  37.773   6.269  1.00 21.05
ATOM   2913  N   GLY   382      16.174  39.874   6.567  1.00 21.33
ATOM   2914  CA  GLY   382      16.561  39.965   5.175  1.00 22.63
ATOM   2915  C   GLY   382      17.670  38.954   4.903  1.00 23.10
ATOM   2916  O   GLY   382      17.708  38.319   3.832  1.00 23.74
ATOM   2917  N   VAL   383      18.579  38.778   5.859  1.00 21.83
ATOM   2918  CA  VAL   383      19.642  37.828   5.615  1.00 22.47
ATOM   2919  CB  VAL   383      20.786  37.967   6.643  1.00 22.80
ATOM   2920  CG1 VAL   383      21.737  36.777   6.525  1.00 21.04
ATOM   2921  CG2 VAL   383      21.562  39.298   6.396  1.00 21.85
ATOM   2922  C   VAL   383      19.075  36.423   5.639  1.00 22.92
ATOM   2923  O   VAL   383      19.199  35.681   4.675  1.00 23.65
ATOM   2924  N   ILE   384      18.414  36.061   6.724  1.00 23.52
ATOM   2925  CA  ILE   384      17.853  34.721   6.835  1.00 24.64
ATOM   2926  CB  ILE   384      17.124  34.551   8.179  1.00 24.17
ATOM   2927  CG2 ILE   384      16.533  33.143   8.283  1.00 22.50
ATOM   2928  CG1 ILE   384      18.112  34.810   9.318  1.00 23.69
ATOM   2929  CD1 ILE   384      17.476  34.861  10.661  1.00 24.39
ATOM   2930  C   ILE   384      16.910  34.324   5.691  1.00 26.04
ATOM   2931  O   ILE   384      17.029  33.233   5.144  1.00 26.98
ATOM   2932  N   ASN   385      15.974  35.182   5.310  1.00 26.88
ATOM   2933  CA  ASN   385      15.097  34.785   4.218  1.00 27.99
ATOM   2934  CB  ASN   385      13.984  35.819   3.998  1.00 25.92
ATOM   2935  CG  ASN   385      13.038  35.918   5.174  1.00 23.68
ATOM   2936  OD1 ASN   385      12.721  34.921   5.820  1.00 21.60
ATOM   2937  ND2 ASN   385      12.567  37.128   5.448  1.00 23.03
ATOM   2938  C   ASN   385      15.888  34.579   2.915  1.00 29.62
ATOM   2939  O   ASN   385      15.610  33.647   2.143  1.00 29.62
ATOM   2940  N   ARG   386      16.869  35.440   2.660  1.00 31.30
ATOM   2941  CA  ARG   386      17.660  35.301   1.442  1.00 33.07
ATOM   2942  CB  ARG   386      18.840  36.261   1.446  1.00 32.62
ATOM   2943  CG  ARG   386      19.697  36.147   0.214  1.00 33.28
ATOM   2944  CD  ARG   386      20.908  37.059   0.284  1.00 34.52
ATOM   2945  NE  ARG   386      21.923  36.698  -0.704  1.00 35.29
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Figure 4

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ATOM   2946  CZ  ARG   386      21.812  36.910  -2.014  1.00 36.32
ATOM   2947  NH1 ARG   386      20.729  37.492  -2.518  1.00 35.95
ATOM   2948  NH2 ARG   386      22.782  36.525  -2.832  1.00 37.07
ATOM   2949  C   ARG   386      18.178  33.875   1.362  1.00 34.69
ATOM   2950  O   ARG   386      18.077  33.232   0.320  1.00 35.70
ATOM   2951  N   MSE   387      18.710  33.383   2.480  1.00 35.94
ATOM   2952  CA  MSE   387      19.250  32.036   2.560  1.00 37.39
ATOM   2953  CB  MSE   387      19.903  31.828   3.927  1.00 39.78
ATOM   2954  CG  MSE   387      21.099  32.754   4.186  1.00 42.37
ATOM   2955  SE  MSE   387      21.873  32.552   5.859  1.00 49.18
ATOM   2956  CE  MSE   387      21.738  30.694   6.097  1.00 44.67
ATOM   2957  C   MSE   387      18.179  30.976   2.311  1.00 38.50
ATOM   2958  O   MSE   387      18.463  29.927   1.721  1.00 37.80
ATOM   2959  N   ARG   388      16.954  31.255   2.769  1.00 40.15
ATOM   2960  CA  ARG   388      15.808  30.352   2.586  1.00 41.28
ATOM   2961  CB  ARG   388      14.554  30.941   3.245  1.00 42.50
ATOM   2962  CG  ARG   388      13.268  30.115   3.069  1.00 42.73
ATOM   2963  CD  ARG   388      12.266  30.443   4.178  1.00 43.15
ATOM   2964  NE  ARG   388      10.965  29.787   4.012  1.00 44.47
ATOM   2965  CZ  ARG   388      10.049  30.134   3.104  1.00 44.46
ATOM   2966  NH1 ARG   388      10.283  31.139   2.269  1.00 44.11
ATOM   2967  NH2 ARG   388       8.895  29.478   3.033  1.00 44.15
ATOM   2968  C   ARG   388      15.579  30.210   1.094  1.00 41.39
ATOM   2969  O   ARG   388      15.516  29.104   0.554  1.00 40.76
ATOM   2970  N   GLU   389      15.460  31.355   0.439  1.00 41.88
ATOM   2971  CA  GLU   389      15.275  31.405  -0.997  1.00 43.37
ATOM   2972  CB  GLU   389      15.211  32.867  -1.448  1.00 45.21
ATOM   2973  CG  GLU   389      15.227  33.079  -2.957  1.00 48.22
ATOM   2974  CD  GLU   389      13.894  32.754  -3.632  1.00 50.35
ATOM   2975  OE1 GLU   389      13.850  32.799  -4.891  1.00 51.00
ATOM   2976  OE2 GLU   389      12.900  32.464  -2.912  1.00 50.86
ATOM   2977  C   GLU   389      16.476  30.713  -1.635  1.00 43.77
ATOM   2978  O   GLU   389      16.325  29.726  -2.355  1.00 43.53
ATOM   2979  N   SER   390      17.671  31.227  -1.335  1.00 43.84
ATOM   2980  CA  SER   390      18.925  30.697  -1.878  1.00 43.61
ATOM   2981  CB  SER   390      20.112  31.549  -1.425  1.00 43.41
ATOM   2982  OG  SER   390      20.229  32.703  -2.241  1.00 43.45
ATOM   2983  C   SER   390      19.243  29.234  -1.607  1.00 43.62
ATOM   2984  O   SER   390      20.126  28.671  -2.251  1.00 44.11
ATOM   2985  N   ARG   391      18.555  28.614  -0.660  1.00 43.22
ATOM   2986  CA  ARG   391      18.815  27.213  -0.396  1.00 43.67
ATOM   2987  CB  ARG   391      19.174  26.994   1.078  1.00 42.72
ATOM   2988  CG  ARG   391      20.440  27.699   1.512  1.00 41.51
ATOM   2989  CD  ARG   391      20.907  27.245   2.892  1.00 39.51
ATOM   2990  NE  ARG   391      22.183  27.864   3.231  1.00 37.99
ATOM   2991  CZ  ARG   391      22.940  27.512   4.266  1.00 37.81
ATOM   2992  NH1 ARG   391      22.545  26.540   5.070  1.00 36.05
ATOM   2993  NH2 ARG   391      24.105  28.121   4.482  1.00 37.12
ATOM   2994  C   ARG   391      17.578  26.404  -0.756  1.00 44.95
ATOM   2995  O   ARG   391      17.458  25.241  -0.372  1.00 45.05
ATOM   2996  N   SER   392      16.666  27.023  -1.502  1.00 46.71
ATOM   2997  CA  SER   392      15.420  26.367  -1.895  1.00 48.25
ATOM   2998  CB  SER   392      15.631  25.468  -3.121  1.00 48.10
ATOM   2999  OG  SER   392      15.610  26.216  -4.326  1.00 48.60
ATOM   3000  C   SER   392      14.880  25.536  -0.737  1.00 49.61
ATOM   3001  O   SER   392      14.601  24.344  -0.882  1.00 49.37
ATOM   3002  N   GLU   393      14.749  26.175   0.420  1.00 51.58
ATOM   3003  CA  GLU   393      14.237  25.510   1.617  1.00 53.54
ATOM   3004  CB  GLU   393      15.085  25.897   2.842  1.00 54.33
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Figure 4

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ATOM   3005  CG  GLU   393      16.586  25.655   2.701  1.00 54.92
ATOM   3006  CD  GLU   393      17.057  24.420   3.450  1.00 55.87
ATOM   3007  OE1 GLU   393      16.845  24.347   4.683  1.00 55.29
ATOM   3008  OE2 GLU   393      17.646  23.523   2.806  1.00 56.69
ATOM   3009  C   GLU   393      12.793  25.961   1.838  1.00 54.20
ATOM   3010  O   GLU   393      12.482  27.151   1.693  1.00 53.70
ATOM   3011  N   ASP   394      11.907  25.026   2.173  1.00 55.42
ATOM   3012  CA  ASP   394      10.519  25.404   2.419  1.00 56.88
ATOM   3013  CB  ASP   394       9.585  24.194   2.400  1.00 58.69
ATOM   3014  CG  ASP   394       8.111  24.602   2.415  1.00 61.23
ATOM   3015  OD1 ASP   394       7.691  25.298   3.376  1.00 62.29
ATOM   3016  OD2 ASP   394       7.374  24.237   1.466  1.00 62.03
ATOM   3017  C   ASP   394      10.489  26.041   3.795  1.00 56.57
ATOM   3018  O   ASP   394      10.023  27.164   3.959  1.00 56.22
ATOM   3019  N   VAL   395      10.994  25.298   4.773  1.00 56.79
ATOM   3020  CA  VAL   395      11.086  25.756   6.153  1.00 57.23
ATOM   3021  CB  VAL   395      10.166  24.949   7.093  1.00 57.72
ATOM   3022  CG1 VAL   395      10.444  25.320   8.548  1.00 57.64
ATOM   3023  CG2 VAL   395       8.708  25.221   6.749  1.00 58.46
ATOM   3024  C   VAL   395      12.534  25.538   6.575  1.00 57.01
ATOM   3025  O   VAL   395      12.968  24.407   6.793  1.00 56.90
ATOM   3026  N   MSE   396      13.280  26.626   6.690  1.00 56.80
ATOM   3027  CA  MSE   396      14.682  26.536   7.058  1.00 56.12
ATOM   3028  CB  MSE   396      15.463  27.645   6.375  1.00 57.66
ATOM   3029  CG  MSE   396      16.932  27.623   6.690  1.00 60.51
ATOM   3030  SE  MSE   396      17.716  29.077   6.002  1.00 65.26
ATOM   3031  CE  MSE   396      17.988  28.564   4.293  1.00 64.74
ATOM   3032  C   MSE   396      14.964  26.600   8.545  1.00 54.59
ATOM   3033  O   MSE   396      14.487  27.491   9.245  1.00 54.08
ATOM   3034  N   ARG   397      15.740  25.637   9.025  1.00 53.05
ATOM   3035  CA  ARG   397      16.134  25.613  10.426  1.00 51.13
ATOM   3036  CB  ARG   397      16.226  24.181  10.951  1.00 52.77
ATOM   3037  CG  ARG   397      14.888  23.520  11.244  1.00 55.36
ATOM   3038  CD  ARG   397      15.132  22.079  11.671  1.00 58.69
ATOM   3039  NE  ARG   397      13.985  21.448  12.326  1.00 61.28
ATOM   3040  CZ  ARG   397      14.056  20.294  12.990  1.00 62.10
ATOM   3041  NH1 ARG   397      15.215  19.651  13.078  1.00 62.57
ATOM   3042  NH2 ARG   397      12.978  19.793  13.583  1.00 62.49
ATOM   3043  C   ARG   397      17.509  26.252  10.397  1.00 48.33
ATOM   3044  O   ARG   397      18.273  26.029   9.466  1.00 47.77
ATOM   3045  N   ILE   398      17.825  27.064  11.395  1.00 45.82
ATOM   3046  CA  ILE   398      19.120  27.721  11.396  1.00 43.01
ATOM   3047  CB  ILE   398      19.202  28.791  10.293  1.00 43.25
ATOM   3048  CG2 ILE   398      18.161  29.864  10.532  1.00 43.18
ATOM   3049  CG1 ILE   398      20.594  29.417  10.279  1.00 43.75
ATOM   3050  CD1 ILE   398      20.768  30.466   9.206  1.00 44.64
ATOM   3051  C   ILE   398      19.441  28.381  12.717  1.00 40.64
ATOM   3052  O   ILE   398      18.557  28.890  13.404  1.00 40.10
ATOM   3053  N   THR   399      20.722  28.360  13.060  1.00 37.78
ATOM   3054  CA  THR   399      21.185  28.954  14.290  1.00 35.36
ATOM   3055  CB  THR   399      22.052  27.988  15.079  1.00 35.02
ATOM   3056  OG1 THR   399      21.280  26.832  15.425  1.00 34.92
ATOM   3057  CG2 THR   399      22.570  28.666  16.345  1.00 34.73
ATOM   3058  C   THR   399      22.001  30.197  13.994  1.00 34.71
ATOM   3059  O   THR   399      22.736  30.254  13.005  1.00 35.10
ATOM   3060  N   VAL   400      21.858  31.184  14.871  1.00 32.96
ATOM   3061  CA  VAL   400      22.539  32.457  14.759  1.00 31.07
ATOM   3062  CB  VAL   400      21.514  33.593  14.592  1.00 31.21
ATOM   3063  CG1 VAL   400      22.211  34.934  14.415  1.00 31.76
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Figure 4


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ATOM   3064  CG2 VAL   400      20.628  33.298  13.405  1.00 31.47
ATOM   3065  C   VAL   400      23.336  32.685  16.039  1.00 30.19
ATOM   3066  O   VAL   400      22.779  32.640  17.144  1.00 30.96
ATOM   3067  N   GLY   401      24.641  32.905  15.888  1.00 28.35
ATOM   3068  CA  GLY   401      25.482  33.150  17.041  1.00 24.47
ATOM   3069  C   GLY   401      25.487  34.641  17.235  1.00 23.04
ATOM   3070  O   GLY   401      25.595  35.388  16.260  1.00 20.38
ATOM   3071  N   VAL   402      25.367  35.086  18.482  1.00 23.36
ATOM   3072  CA  VAL   402      25.338  36.514  18.751  1.00 23.38
ATOM   3073  CB  VAL   402      23.927  36.960  19.124  1.00 22.79
ATOM   3074  CG1 VAL   402      23.790  38.458  18.909  1.00 22.85
ATOM   3075  CG2 VAL   402      22.895  36.176  18.320  1.00 22.42
ATOM   3076  C   VAL   402      26.252  36.899  19.893  1.00 24.25
ATOM   3077  O   VAL   402      26.484  36.098  20.794  1.00 25.20
ATOM   3078  N   ASP   403      26.770  38.124  19.848  1.00 24.83
ATOM   3079  CA  ASP   403      27.637  38.649  20.894  1.00 27.11
ATOM   3080  CB  ASP   403      29.078  38.212  20.691  1.00 30.98
ATOM   3081  CG  ASP   403      30.003  38.739  21.787  1.00 34.48
ATOM   3082  OD1 ASP   403      29.887  39.938  22.122  1.00 36.02
ATOM   3083  OD2 ASP   403      30.842  37.960  22.311  1.00 36.05
ATOM   3084  C   ASP   403      27.562  40.154  20.763  1.00 27.24
ATOM   3085  O   ASP   403      27.550  40.667  19.645  1.00 29.15
ATOM   3086  N   GLY   404      27.519  40.863  21.888  1.00 26.60
ATOM   3087  CA  GLY   404      27.410  42.316  21.863  1.00 26.50
ATOM   3088  C   GLY   404      26.750  42.829  23.137  1.00 27.10
ATOM   3089  O   GLY   404      25.810  42.193  23.665  1.00 26.90
ATOM   3090  N   SER   405      27.209  43.972  23.644  1.00 26.72
ATOM   3091  CA  SER   405      26.638  44.496  24.887  1.00 27.96
ATOM   3092  CB  SER   405      27.409  45.722  25.371  1.00 28.04
ATOM   3093  OG  SER   405      27.164  46.828  24.521  1.00 30.53
ATOM   3094  C   SER   405      25.168  44.857  24.738  1.00 28.25
ATOM   3095  O   SER   405      24.341  44.473  25.573  1.00 27.96
ATOM   3096  N   VAL   406      24.844  45.591  23.675  1.00 27.79
ATOM   3097  CA  VAL   406      23.465  45.992  23.445  1.00 28.13
ATOM   3098  CB  VAL   406      23.281  46.667  22.074  1.00 28.02
ATOM   3099  CG1 VAL   406      21.814  47.063  21.908  1.00 27.91
ATOM   3100  CG2 VAL   406      24.197  47.877  21.940  1.00 26.07
ATOM   3101  C   VAL   406      22.535  44.789  23.488  1.00 28.35
ATOM   3102  O   VAL   406      21.484  44.826  24.120  1.00 28.48
ATOM   3103  N   TYR   407      22.934  43.718  22.811  1.00 28.72
ATOM   3104  CA  TYR   407      22.130  42.493  22.736  1.00 28.45
ATOM   3105  CB  TYR   407      22.613  41.643  21.558  1.00 26.86
ATOM   3106  CG  TYR   407      21.831  40.373  21.341  1.00 25.29
ATOM   3107  CD1 TYR   407      20.700  40.358  20.535  1.00 25.44
ATOM   3108  CE1 TYR   407      19.964  39.189  20.346  1.00 25.93
ATOM   3109  CD2 TYR   407      22.213  39.192  21.955  1.00 24.93
ATOM   3110  CE2 TYR   407      21.488  38.021  21.780  1.00 25.18
ATOM   3111  CZ  TYR   407      20.362  38.024  20.974  1.00 26.03
ATOM   3112  OH  TYR   407      19.626  36.868  20.822  1.00 25.67
ATOM   3113  C   TYR   407      22.175  41.651  24.014  1.00 28.83
ATOM   3114  O   TYR   407      21.202  40.988  24.369  1.00 28.62
ATOM   3115  N   LYS   408      23.306  41.674  24.705  1.00 29.64
ATOM   3116  CA  LYS   408      23.440  40.881  25.916  1.00 30.07
ATOM   3117  CB  LYS   408      24.904  40.477  26.118  1.00 30.08
ATOM   3118  CG  LYS   408      25.442  39.556  25.030  1.00 30.61
ATOM   3119  CD  LYS   408      26.597  38.698  25.529  1.00 30.05
ATOM   3120  CE  LYS   408      26.799  37.515  24.601  1.00 30.22
ATOM   3121  NZ  LYS   408      27.828  36.573  25.097  1.00 30.20
ATOM   3122  C   LYS   408      22.940  41.551  27.185  1.00 30.82
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Figure 4

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ATOM   3123  O   LYS  408      22.327  40.901  28.038  1.00 31.98
ATOM   3124  N   LEU  409      23.176  42.853  27.296  1.00 30.97
ATOM   3125  CA  LEU  409      22.823  43.598  28.501  1.00 31.11
ATOM   3126  CB  LEU  409      24.006  44.482  28.875  1.00 30.54
ATOM   3127  CG  LEU  409      25.305  43.700  28.962  1.00 29.31
ATOM   3128  CD1 LEU  409      26.372  44.591  29.597  1.00 29.41
ATOM   3129  CD2 LEU  409      25.067  42.423  29.785  1.00 28.16
ATOM   3130  C   LEU  409      21.548  44.441  28.611  1.00 31.44
ATOM   3131  O   LEU  409      20.978  44.542  29.708  1.00 31.86
ATOM   3132  N   HIS  410      21.122  45.077  27.519  1.00 31.34
ATOM   3133  CA  HIS  410      19.929  45.912  27.572  1.00 30.80
ATOM   3134  CB  HIS  410      19.732  46.635  26.247  1.00 30.36
ATOM   3135  CG  HIS  410      18.703  47.717  26.303  1.00 29.89
ATOM   3136  CD2 HIS  410      18.815  49.060  26.179  1.00 29.29
ATOM   3137  ND1 HIS  410      17.362  47.457  26.508  1.00 30.79
ATOM   3138  CE1 HIS  410      16.691  48.595  26.505  1.00 29.88
ATOM   3139  NE2 HIS  410      17.548  49.583  26.309  1.00 30.87
ATOM   3140  C   HIS  410      18.728  45.031  27.900  1.00 31.41
ATOM   3141  O   HIS  410      18.467  44.055  27.207  1.00 31.97
ATOM   3142  N   PRO  411      17.985  45.376  28.969  1.00 31.63
ATOM   3143  CD  PRO  411      18.173  46.690  29.610  1.00 31.32
ATOM   3144  CA  PRO  411      16.798  44.708  29.518  1.00 31.33
ATOM   3145  CB  PRO  411      16.111  45.815  30.299  1.00 31.27
ATOM   3146  CG  PRO  411      17.257  46.599  30.822  1.00 32.32
ATOM   3147  C   PRO  411      15.827  44.037  28.571  1.00 32.09
ATOM   3148  O   PRO  411      15.362  42.920  28.838  1.00 32.76
ATOM   3149  N   SER  412      15.519  44.684  27.457  1.00 31.73
ATOM   3150  CA  SER  412      14.527  44.094  26.573  1.00 31.92
ATOM   3151  CB  SER  412      13.210  44.834  26.771  1.00 32.51
ATOM   3152  OG  SER  412      13.368  46.200  26.390  1.00 33.27
ATOM   3153  C   SER  412      14.838  44.047  25.082  1.00 31.91
ATOM   3154  O   SER  412      14.039  43.520  24.304  1.00 32.59
ATOM   3155  N   PHE  413      15.974  44.601  24.679  1.00 30.72
ATOM   3156  CA  PHE  413      16.348  44.615  23.271  1.00 30.13
ATOM   3157  CB  PHE  413      17.778  45.105  23.130  1.00 28.18
ATOM   3158  CG  PHE  413      18.213  45.285  21.716  1.00 25.96
ATOM   3159  CD1 PHE  413      18.085  46.522  21.094  1.00 25.70
ATOM   3160  CD2 PHE  413      18.772  44.233  21.015  1.00 24.47
ATOM   3161  CE1 PHE  413      18.517  46.711  19.787  1.00 25.13
ATOM   3162  CE2 PHE  413      19.208  44.408  19.707  1.00 24.84
ATOM   3163  CZ  PHE  413      19.082  45.652  19.092  1.00 24.48
ATOM   3164  C   PHE  413      16.232  43.228  22.645  1.00 31.20
ATOM   3165  O   PHE  413      15.571  43.026  21.612  1.00 31.56
ATOM   3166  N   LYS  414      16.888  42.268  23.275  1.00 31.75
ATOM   3167  CA  LYS  414      16.851  40.906  22.790  1.00 32.75
ATOM   3168  CB  LYS  414      17.626  39.999  23.755  1.00 33.66
ATOM   3169  CG  LYS  414      17.570  38.526  23.429  1.00 34.45
ATOM   3170  CD  LYS  414      18.732  37.744  24.049  1.00 36.05
ATOM   3171  CE  LYS  414      18.845  37.909  25.558  1.00 35.80
ATOM   3172  NZ  LYS  414      19.972  38.817  25.920  1.00 36.66
ATOM   3173  C   LYS  414      15.412  40.411  22.600  1.00 33.19
ATOM   3174  O   LYS  414      15.054  39.927  21.518  1.00 33.30
ATOM   3175  N   GLU  415      14.577  40.542  23.627  1.00 33.81
ATOM   3176  CA  GLU  415      13.193  40.071  23.513  1.00 34.53
ATOM   3177  CB  GLU  415      12.462  40.251  24.838  1.00 37.66
ATOM   3178  CG  GLU  415      13.062  39.497  26.002  1.00 42.83
ATOM   3179  CD  GLU  415      14.376  40.090  26.520  1.00 45.68
ATOM   3180  OE1 GLU  415      14.523  41.339  26.526  1.00 47.31
ATOM   3181  OE2 GLU  415      15.245  39.293  26.956  1.00 47.44
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Figure 4

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ATOM   3182  C   GLU 415      12.409  40.776  22.401  1.00 33.23
ATOM   3183  O   GLU 415      11.676  40.137  21.649  1.00 33.06
ATOM   3184  N   ARG 416      12.551  42.092  22.299  1.00 31.77
ATOM   3185  CA  ARG 416      11.841  42.825  21.264  1.00 30.32
ATOM   3186  CB  ARG 416      12.066  44.328  21.427  1.00 31.27
ATOM   3187  CG  ARG 416      11.645  44.875  22.796  1.00 33.92
ATOM   3188  CD  ARG 416      11.783  46.393  22.901  1.00 35.48
ATOM   3189  NE  ARG 416      11.545  46.866  24.267  1.00 38.24
ATOM   3190  CZ  ARG 416      11.982  48.030  24.746  1.00 39.11
ATOM   3191  NH1 ARG 416      12.676  48.850  23.967  1.00 39.89
ATOM   3192  NH2 ARG 416      11.754  48.365  26.009  1.00 38.52
ATOM   3193  C   ARG 416      12.379  42.354  19.916  1.00 29.08
ATOM   3194  O   ARG 416      11.620  42.159  18.964  1.00 28.85
ATOM   3195  N   PHE 417      13.694  42.144  19.862  1.00 27.59
ATOM   3196  CA  PHE 417      14.377  41.707  18.648  1.00 25.70
ATOM   3197  CB  PHE 417      15.886  41.687  18.890  1.00 23.64
ATOM   3198  CG  PHE 417      16.687  41.310  17.680  1.00 20.59
ATOM   3199  CD1 PHE 417      16.910  42.230  16.671  1.00 18.99
ATOM   3200  CD2 PHE 417      17.183  40.018  17.540  1.00 19.41
ATOM   3201  CE1 PHE 417      17.610  41.870  15.540  1.00 19.87
ATOM   3202  CE2 PHE 417      17.884  39.641  16.413  1.00 18.04
ATOM   3203  CZ  PHE 417      18.100  40.563  15.409  1.00 20.04
ATOM   3204  C   PHE 417      13.943  40.342  18.099  1.00 25.74
ATOM   3205  O   PHE 417      13.568  40.225  16.927  1.00 25.24
ATOM   3206  N   HIS 418      14.012  39.301  18.922  1.00 26.11
ATOM   3207  CA  HIS 418      13.612  37.962  18.459  1.00 26.79
ATOM   3208  CB  HIS 418      13.638  36.973  19.615  1.00 28.01
ATOM   3209  CG  HIS 418      14.973  36.854  20.279  1.00 28.81
ATOM   3210  CD2 HIS 418      16.168  37.425  19.989  1.00 29.42
ATOM   3211  ND1 HIS 418      15.182  36.067  21.389  1.00 28.15
ATOM   3212  CE1 HIS 418      16.446  36.157  21.755  1.00 29.43
ATOM   3213  NE2 HIS 418      17.067  36.974  20.924  1.00 29.74
ATOM   3214  C   HIS 418      12.209  37.985  17.876  1.00 26.41
ATOM   3215  O   HIS 418      11.976  37.565  16.733  1.00 26.40
ATOM   3216  N   ALA 419      11.284  38.487  18.688  1.00 25.83
ATOM   3217  CA  ALA 419       9.885  38.603  18.328  1.00 25.05
ATOM   3218  CB  ALA 419       9.182  39.454  19.352  1.00 24.80
ATOM   3219  C   ALA 419       9.781  39.215  16.943  1.00 25.35
ATOM   3220  O   ALA 419       9.146  38.601  16.029  1.00 25.99
ATOM   3221  N   SER 420      10.249  40.425  16.777  1.00 25.26
ATOM   3222  CA  SER 420      10.159  41.078  15.481  1.00 25.31
ATOM   3223  CB  SER 420      10.897  42.405  15.515  1.00 23.85
ATOM   3224  OG  SER 420      10.692  43.089  14.303  1.00 23.43
ATOM   3225  C   SER 420      10.751  40.170  14.391  1.00 26.14
ATOM   3226  O   SER 420      10.145  39.976  13.331  1.00 25.95
ATOM   3227  N   VAL 421      11.926  39.602  14.670  1.00 27.34
ATOM   3228  CA  VAL 421      12.602  38.699  13.733  1.00 28.41
ATOM   3229  CB  VAL 421      13.919  38.127  14.346  1.00 27.63
ATOM   3230  CG1 VAL 421      14.479  37.020  13.475  1.00 26.36
ATOM   3231  CG2 VAL 421      14.953  39.232  14.469  1.00 28.22
ATOM   3232  C   VAL 421      11.689  37.535  13.325  1.00 29.65
ATOM   3233  O   VAL 421      11.557  37.227  12.130  1.00 28.72
ATOM   3234  N   ARG 422      11.069  36.886  14.310  1.00 30.74
ATOM   3235  CA  ARG 422      10.165  35.775  14.014  1.00 32.79
ATOM   3236  CB  ARG 422       9.419  35.328  15.265  1.00 33.29
ATOM   3237  CG  ARG 422      10.259  35.197  16.512  1.00 34.47
ATOM   3238  CD  ARG 422      11.081  33.927  16.558  1.00 34.54
ATOM   3239  NE  ARG 422      11.862  33.905  17.795  1.00 35.75
ATOM   3240  CZ  ARG 422      12.824  33.028  18.066  1.00 35.45
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ATOM   3241  NH1 ARG   422      13.127  32.085  17.180  1.00 35.35
ATOM   3242  NH2 ARG   422      13.490  33.108  19.215  1.00 33.55
ATOM   3243  C   ARG   422       9.123  36.277  13.019  1.00 33.41
ATOM   3244  O   ARG   422       8.949  35.728  11.929  1.00 33.68
ATOM   3245  N   ARG   423       8.446  37.348  13.417  1.00 34.00
ATOM   3246  CA  ARG   423       7.394  37.946  12.622  1.00 34.13
ATOM   3247  CB  ARG   423       7.022  39.301  13.207  1.00 35.16
ATOM   3248  CG  ARG   423       5.538  39.584  13.202  1.00 36.10
ATOM   3249  CD  ARG   423       5.212  40.831  14.012  1.00 37.57
ATOM   3250  NE  ARG   423       5.482  40.682  15.441  1.00 38.90
ATOM   3251  CZ  ARG   423       6.274  41.503  16.133  1.00 40.51
ATOM   3252  NH1 ARG   423       6.874  42.523  15.513  1.00 41.42
ATOM   3253  NH2 ARG   423       6.461  41.324  17.440  1.00 38.76
ATOM   3254  C   ARG   423       7.754  38.100  11.165  1.00 33.94
ATOM   3255  O   ARG   423       6.919  37.849  10.295  1.00 35.59
ATOM   3256  N   LEU   424       8.993  38.494  10.884  1.00 32.85
ATOM   3257  CA  LEU   424       9.418  38.699   9.497  1.00 31.57
ATOM   3258  CB  LEU   424      10.474  39.788   9.450  1.00 28.75
ATOM   3259  CG  LEU   424      10.030  41.129  10.003  1.00 27.64
ATOM   3260  CD1 LEU   424      11.220  42.080  10.066  1.00 26.47
ATOM   3261  CD2 LEU   424       8.942  41.686   9.115  1.00 27.23
ATOM   3262  C   LEU   424       9.950  37.479   8.747  1.00 32.00
ATOM   3263  O   LEU   424      10.232  37.562   7.551  1.00 31.15
ATOM   3264  N   THR   425      10.065  36.343   9.424  1.00 33.88
ATOM   3265  CA  THR   425      10.615  35.153   8.778  1.00 35.30
ATOM   3266  CB  THR   425      11.886  34.722   9.495  1.00 35.17
ATOM   3267  OG1 THR   425      11.580  34.463  10.874  1.00 35.24
ATOM   3268  CG2 THR   425      12.939  35.817   9.399  1.00 35.16
ATOM   3269  C   THR   425       9.711  33.923   8.675  1.00 37.00
ATOM   3270  O   THR   425      10.059  32.854   9.182  1.00 37.54
ATOM   3271  N   PRO   426       8.562  34.040   7.982  1.00 38.04
ATOM   3272  CD  PRO   426       8.144  35.123   7.073  1.00 38.49
ATOM   3273  CA  PRO   426       7.663  32.890   7.856  1.00 38.85
ATOM   3274  CB  PRO   426       6.745  33.295   6.700  1.00 38.23
ATOM   3275  CG  PRO   426       6.699  34.772   6.802  1.00 38.07
ATOM   3276  C   PRO   426       8.445  31.615   7.527  1.00 39.83
ATOM   3277  O   PRO   426       9.378  31.641   6.728  1.00 40.28
ATOM   3278  N   SER   427       8.073  30.510   8.158  1.00 40.72
ATOM   3279  CA  SER   427       8.713  29.232   7.892  1.00 41.82
ATOM   3280  CB  SER   427       8.358  28.785   6.474  1.00 42.86
ATOM   3281  OG  SER   427       6.954  28.802   6.287  1.00 44.69
ATOM   3282  C   SER   427      10.234  29.228   8.068  1.00 42.10
ATOM   3283  O   SER   427      10.981  28.899   7.140  1.00 41.85
ATOM   3284  N   CYS   428      10.679  29.586   9.267  1.00 42.60
ATOM   3285  CA  CYS   428      12.096  29.608   9.601  1.00 42.43
ATOM   3286  CB  CYS   428      12.724  30.960   9.258  1.00 42.59
ATOM   3287  SG  CYS   428      12.860  31.327   7.492  1.00 44.02
ATOM   3288  C   CYS   428      12.195  29.381  11.096  1.00 42.45
ATOM   3289  O   CYS   428      11.671  30.169  11.879  1.00 43.76
ATOM   3290  N   GLU   429      12.846  28.296  11.494  1.00 42.34
ATOM   3291  CA  GLU   429      13.014  27.995  12.909  1.00 41.23
ATOM   3292  CB  GLU   429      13.030  26.486  13.146  1.00 42.97
ATOM   3293  CG  GLU   429      11.699  25.796  12.933  1.00 45.48
ATOM   3294  CD  GLU   429      11.847  24.282  12.925  1.00 47.43
ATOM   3295  OE1 GLU   429      12.518  23.756  13.847  1.00 48.77
ATOM   3296  OE2 GLU   429      11.298  23.623  12.005  1.00 48.07
ATOM   3297  C   GLU   429      14.341  28.587  13.346  1.00 39.77
ATOM   3298  O   GLU   429      15.370  27.902  13.352  1.00 39.92
ATOM   3299  N   ILE   430      14.315  29.864  13.708  1.00 38.09
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ATOM	3300	CA	ILE	430	15.514	30.560	14.142	1.00	36.48
ATOM	3301	CB	ILE	430	15.341	32.070	13.998	1.00	35.17
ATOM	3302	CG2	ILE	430	16.659	32.770	14.280	1.00	34.48
ATOM	3303	CG1	ILE	430	14.839	32.390	12.589	1.00	35.30
ATOM	3304	CD1	ILE	430	14.669	33.866	12.310	1.00	34.88
ATOM	3305	C	ILE	430	15.872	30.254	15.591	1.00	37.06
ATOM	3306	O	ILE	430	15.044	30.399	16.495	1.00	38.13
ATOM	3307	N	THR	431	17.109	29.823	15.808	1.00	36.61
ATOM	3308	CA	THR	431	17.600	29.520	17.146	1.00	36.17
ATOM	3309	CB	THR	431	18.067	28.053	17.240	1.00	36.58
ATOM	3310	OG1	THR	431	16.950	27.180	17.031	1.00	36.34
ATOM	3311	CG2	THR	431	18.692	27.774	18.604	1.00	36.38
ATOM	3312	C	THR	431	18.796	30.441	17.396	1.00	36.13
ATOM	3313	O	THR	431	19.705	30.513	16.569	1.00	36.10
ATOM	3314	N	PHE	432	18.804	31.157	18.514	1.00	35.79
ATOM	3315	CA	PHE	432	19.926	32.054	18.794	1.00	35.93
ATOM	3316	CB	PHE	432	19.443	33.450	19.232	1.00	34.31
ATOM	3317	CG	PHE	432	18.643	34.194	18.188	1.00	32.53
ATOM	3318	CD1	PHE	432	17.271	33.977	18.048	1.00	31.59
ATOM	3319	CD2	PHE	432	19.262	35.124	17.353	1.00	31.00
ATOM	3320	CE1	PHE	432	16.527	34.676	17.092	1.00	30.53
ATOM	3321	CE2	PHE	432	18.525	35.826	16.395	1.00	30.25
ATOM	3322	CZ	PHE	432	17.154	35.600	16.266	1.00	30.11
ATOM	3323	C	PHE	432	20.767	31.483	19.917	1.00	37.08
ATOM	3324	O	PHE	432	20.248	30.772	20.779	1.00	38.85
ATOM	3325	N	ILE	433	22.063	31.774	19.906	1.00	37.32
ATOM	3326	CA	ILE	433	22.933	31.321	20.983	1.00	38.46
ATOM	3327	CB	ILE	433	23.526	29.890	20.722	1.00	39.06
ATOM	3328	CG2	ILE	433	22.398	28.863	20.624	1.00	38.62
ATOM	3329	CG1	ILE	433	24.367	29.861	19.449	1.00	39.03
ATOM	3330	CD1	ILE	433	25.028	28.520	19.227	1.00	38.32
ATOM	3331	C	ILE	433	24.039	32.358	21.161	1.00	39.33
ATOM	3332	O	ILE	433	24.429	33.034	20.201	1.00	39.15
ATOM	3333	N	GLU	434	24.527	32.505	22.388	1.00	40.58
ATOM	3334	CA	GLU	434	25.559	33.498	22.669	1.00	42.92
ATOM	3335	CB	GLU	434	25.152	34.312	23.885	1.00	43.91
ATOM	3336	CG	GLU	434	23.769	34.883	23.744	1.00	45.53
ATOM	3337	CD	GLU	434	23.342	35.640	24.965	1.00	46.68
ATOM	3338	OE1	GLU	434	23.436	35.072	26.074	1.00	47.18
ATOM	3339	OE2	GLU	434	22.910	36.802	24.816	1.00	48.77
ATOM	3340	C	GLU	434	26.965	32.950	22.865	1.00	44.01
ATOM	3341	O	GLU	434	27.206	32.058	23.680	1.00	44.48
ATOM	3342	N	SER	435	27.901	33.518	22.119	1.00	45.00
ATOM	3343	CA	SER	435	29.284	33.075	22.167	1.00	46.11
ATOM	3344	CB	SER	435	30.077	33.779	21.057	1.00	46.95
ATOM	3345	OG	SER	435	29.839	35.186	21.053	1.00	47.94
ATOM	3346	C	SER	435	29.984	33.274	23.507	1.00	46.36
ATOM	3347	O	SER	435	30.043	34.396	24.022	1.00	46.31
ATOM	3348	N	GLU	436	30.505	32.180	24.069	1.00	46.22
ATOM	3349	CA	GLU	436	31.248	32.250	25.330	1.00	46.33
ATOM	3350	CB	GLU	436	31.322	30.884	26.020	1.00	47.64
ATOM	3351	CG	GLU	436	32.144	30.908	27.317	1.00	50.83
ATOM	3352	CD	GLU	436	32.726	29.541	27.711	1.00	52.03
ATOM	3353	OE1	GLU	436	31.951	28.585	27.970	1.00	52.84
ATOM	3354	OE2	GLU	436	33.972	29.428	27.765	1.00	52.07
ATOM	3355	C	GLU	436	32.650	32.671	24.912	1.00	45.58
ATOM	3356	O	GLU	436	33.446	31.843	24.463	1.00	45.50
ATOM	3357	N	GLU	437	32.950	33.956	25.051	1.00	44.67
ATOM	3358	CA	GLU	437	34.252	34.462	24.643	1.00	44.13

Figure 4

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ATOM   3359  CB  GLU  437      35.328  34.050  25.652  1.00 43.61
ATOM   3360  CG  GLU  437      36.745  34.334  25.190  1.00 43.39
ATOM   3361  CD  GLU  437      36.931  35.752  24.678  1.00 43.50
ATOM   3362  OE1 GLU  437      36.976  36.680  25.514  1.00 44.49
ATOM   3363  OE2 GLU  437      37.025  35.940  23.441  1.00 42.17
ATOM   3364  C   GLU  437      34.569  33.880  23.264  1.00 43.56
ATOM   3365  O   GLU  437      35.530  33.131  23.108  1.00 45.30
ATOM   3366  N   GLY  438      33.757  34.225  22.266  1.00 41.68
ATOM   3367  CA  GLY  438      33.958  33.700  20.926  1.00 39.44
ATOM   3368  C   GLY  438      34.748  34.538  19.934  1.00 38.11
ATOM   3369  O   GLY  438      34.932  34.130  18.791  1.00 37.45
ATOM   3370  N   SER  439      35.213  35.713  20.329  1.00 37.14
ATOM   3371  CA  SER  439      35.980  36.502  19.386  1.00 36.86
ATOM   3372  CB  SER  439      35.916  37.983  19.714  1.00 36.81
ATOM   3373  OG  SER  439      36.825  38.678  18.878  1.00 35.32
ATOM   3374  C   SER  439      37.420  36.053  19.444  1.00 36.74
ATOM   3375  O   SER  439      38.192  36.265  18.513  1.00 36.37
ATOM   3376  N   GLY  440      37.774  35.439  20.562  1.00 36.58
ATOM   3377  CA  GLY  440      39.126  34.957  20.746  1.00 36.42
ATOM   3378  C   GLY  440      39.207  33.518  20.302  1.00 36.28
ATOM   3379  O   GLY  440      40.146  33.140  19.613  1.00 36.20
ATOM   3380  N   ARG  441      38.224  32.714  20.699  1.00 36.09
ATOM   3381  CA  ARG  441      38.190  31.309  20.312  1.00 37.16
ATOM   3382  CB  ARG  441      37.151  30.562  21.138  1.00 37.34
ATOM   3383  CG  ARG  441      37.312  30.717  22.632  1.00 39.57
ATOM   3384  CD  ARG  441      36.334  29.806  23.375  1.00 42.28
ATOM   3385  NE  ARG  441      35.270  29.339  22.488  1.00 44.36
ATOM   3386  CZ  ARG  441      34.240  28.585  22.862  1.00 45.80
ATOM   3387  NH1 ARG  441      34.103  28.192  24.127  1.00 45.87
ATOM   3388  NH2 ARG  441      33.346  28.214  21.955  1.00 47.26
ATOM   3389  C   ARG  441      37.848  31.179  18.821  1.00 37.42
ATOM   3390  O   ARG  441      38.103  30.151  18.189  1.00 37.52
ATOM   3391  N   GLY  442      37.270  32.234  18.262  1.00 37.34
ATOM   3392  CA  GLY  442      36.906  32.204  16.863  1.00 37.39
ATOM   3393  C   GLY  442      38.165  32.308  16.048  1.00 37.47
ATOM   3394  O   GLY  442      38.483  31.410  15.278  1.00 37.51
ATOM   3395  N   ALA  443      38.887  33.408  16.241  1.00 38.17
ATOM   3396  CA  ALA  443      40.134  33.660  15.526  1.00 38.50
ATOM   3397  CB  ALA  443      40.739  34.999  15.967  1.00 36.50
ATOM   3398  C   ALA  443      41.127  32.521  15.759  1.00 39.03
ATOM   3399  O   ALA  443      42.015  32.297  14.941  1.00 39.36
ATOM   3400  N   ALA  444      40.977  31.807  16.875  1.00 39.93
ATOM   3401  CA  ALA  444      41.864  30.685  17.172  1.00 40.31
ATOM   3402  CB  ALA  444      41.724  30.242  18.623  1.00 39.25
ATOM   3403  C   ALA  444      41.427  29.569  16.246  1.00 40.97
ATOM   3404  O   ALA  444      42.146  29.210  15.312  1.00 41.31
ATOM   3405  N   LEU  445      40.233  29.038  16.501  1.00 41.41
ATOM   3406  CA  LEU  445      39.678  27.960  15.690  1.00 41.97
ATOM   3407  CB  LEU  445      38.195  27.776  16.024  1.00 40.09
ATOM   3408  CG  LEU  445      37.954  26.806  17.182  1.00 39.14
ATOM   3409  CD1 LEU  445      36.750  27.233  17.982  1.00 39.27
ATOM   3410  CD2 LEU  445      37.781  25.399  16.647  1.00 37.36
ATOM   3411  C   LEU  445      39.860  28.156  14.176  1.00 43.29
ATOM   3412  O   LEU  445      39.918  27.179  13.427  1.00 43.28
ATOM   3413  N   VAL  446      39.955  29.406  13.729  1.00 44.66
ATOM   3414  CA  VAL  446      40.136  29.684  12.307  1.00 46.32
ATOM   3415  CB  VAL  446      39.687  31.120  11.948  1.00 46.15
ATOM   3416  CG1 VAL  446      40.356  31.578  10.653  1.00 46.15
ATOM   3417  CG2 VAL  446      38.164  31.160  11.793  1.00 45.75
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Figure 4

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ATOM   3418  C   VAL   446      41.597  29.503  11.944  1.00 48.03
ATOM   3419  O   VAL   446      41.929  29.105  10.825  1.00 48.75
ATOM   3420  N   SER   447      42.465  29.802  12.904  1.00 49.63
ATOM   3421  CA  SER   447      43.902  29.657  12.725  1.00 50.76
ATOM   3422  CB  SER   447      44.635  30.267  13.918  1.00 50.76
ATOM   3423  OG  SER   447      44.377  31.659  14.021  1.00 50.83
ATOM   3424  C   SER   447      44.259  28.173  12.612  1.00 52.07
ATOM   3425  O   SER   447      44.923  27.753  11.662  1.00 52.17
ATOM   3426  N   ALA   448      43.804  27.387  13.584  1.00 53.51
ATOM   3427  CA  ALA   448      44.071  25.953  13.621  1.00 55.46
ATOM   3428  CB  ALA   448      43.273  25.306  14.745  1.00 55.02
ATOM   3429  C   ALA   448      43.751  25.263  12.300  1.00 57.02
ATOM   3430  O   ALA   448      44.599  24.564  11.726  1.00 57.18
ATOM   3431  N   VAL   449      42.523  25.457  11.825  1.00 58.39
ATOM   3432  CA  VAL   449      42.093  24.841  10.579  1.00 59.69
ATOM   3433  CB  VAL   449      40.571  24.977  10.382  1.00 59.67
ATOM   3434  CG1 VAL   449      40.152  24.262   9.112  1.00 60.28
ATOM   3435  CG2 VAL   449      39.833  24.384  11.577  1.00 59.48
ATOM   3436  C   VAL   449      42.821  25.482   9.403  1.00 60.70
ATOM   3437  O   VAL   449      42.903  24.898   8.321  1.00 61.00
ATOM   3438  N   ALA   450      43.361  26.677   9.627  1.00 61.41
ATOM   3439  CA  ALA   450      44.093  27.392   8.591  1.00 62.12
ATOM   3440  CB  ALA   450      43.981  28.889   8.814  1.00 62.32
ATOM   3441  C   ALA   450      45.558  26.973   8.606  1.00 63.02
ATOM   3442  O   ALA   450      46.437  27.748   8.217  1.00 62.75
ATOM   3443  N   CYS   451      45.807  25.744   9.061  1.00 64.03
ATOM   3444  CA  CYS   451      47.160  25.183   9.148  1.00 65.19
ATOM   3445  CB  CYS   451      47.530  24.440   7.850  1.00 65.75
ATOM   3446  SG  CYS   451      46.901  22.720   7.723  1.00 66.86
ATOM   3447  C   CYS   451      48.239  26.217   9.474  1.00 65.22
ATOM   3448  O   CYS   451      47.929  27.230  10.144  1.00 65.18
ATOM   3449  OXT CYS   451      49.398  25.979   9.073  1.00 65.50
ATOM   3450  C1  HEX     1      31.023  47.521  12.611  1.00 25.83
ATOM   3451  C2  HEX     1      32.239  47.182  11.801  1.00 25.25
ATOM   3452  C3  HEX     1      32.203  45.697  11.565  1.00 25.11
ATOM   3453  C4  HEX     1      32.071  44.939  12.862  1.00 24.99
ATOM   3454  C5  HEX     1      31.030  45.591  13.785  1.00 25.34
ATOM   3455  C6  HEX     1      30.772  44.921  15.126  1.00 25.58
ATOM   3456  O1  HEX     1      30.750  48.942  12.579  1.00 27.04
ATOM   3457  O2  HEX     1      32.183  47.912  10.609  1.00 24.71
ATOM   3458  O3  HEX     1      33.337  45.251  10.836  1.00 25.99
ATOM   3459  O4  HEX     1      31.699  43.621  12.545  1.00 25.85
ATOM   3460  O5  HEX     1      31.267  46.968  13.935  1.00 25.37
ATOM   3461  O6  HEX     1      31.835  45.222  16.009  1.00 27.23
ATOM   3462  C1  LIG     1      30.034  26.620   8.669  1.00 35.87
ATOM   3463  C2  LIG     1      29.909  27.259  10.064  1.00 34.82
ATOM   3464  C3  LIG     1      31.308  27.852  10.344  1.00 35.54
ATOM   3465  C4  LIG     1      32.212  27.447   9.148  1.00 35.52
ATOM   3466  C5  LIG     1      31.520  26.207   8.584  1.00 35.20
ATOM   3467  C6  LIG     1      33.670  27.245   9.637  1.00 36.33
ATOM   3468  C7  LIG     1      34.562  26.321   8.758  1.00 37.11
ATOM   3469  C8  LIG     1      35.946  26.832   8.778  1.00 36.91
ATOM   3470  N9  LIG     1      36.382  27.317   7.570  1.00 36.92
ATOM   3471  C10 LIG     1      37.668  27.907   7.331  1.00 36.42
ATOM   3472  N11 LIG     1      38.035  28.336   6.087  1.00 37.39
ATOM   3473  C12 LIG     1      39.058  28.930   6.462  1.00 36.99
ATOM   3474  C13 LIG     1      39.426  29.003   7.575  1.00 37.10
ATOM   3475  S14 LIG     1      38.681  28.342   8.700  1.00 37.86
ATOM   3476  O15 LIG     1      36.640  26.843   9.817  1.00 38.32
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Figure 4

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ATOM   3477  C16 LIG     1      34.538  24.890   9.296  1.00 37.59
ATOM   3478  C17 LIG     1      34.906  24.620  10.610  1.00 37.22
ATOM   3479  C18 LIG     1      34.658  23.346  11.130  1.00 38.09
ATOM   3480  N19 LIG     1      34.084  22.371  10.404  1.00 38.80
ATOM   3481  C20 LIG     1      33.729  22.598   9.128  1.00 38.90
ATOM   3482  C21 LIG     1      33.942  23.860   8.546  1.00 38.73
ATOM   3483  K1  K       1      32.471  32.037  -7.104  1.00 46.91
END
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CRYSTALS OF GLUCOKINASE AND METHODS OF GROWING THEM

The invention relates to crystalline forms of Glucokinase of sufficient size and quality to obtain structural data by X-ray crystallography and to methods of growing such crystals.

Glucokinase (GK) is one of four hexokinases found in mammals [Colowick, S.P., in *The Enzymes*, Vol. 9 (P. Boyer, ed.) Academic Press, New York, NY, pages 1-48, 1973]. The hexokinases catalyze the first step in the metabolism of glucose, i.e., the conversion of glucose to glucose-6-phosphate. Glucokinase has a limited cellular distribution, being found principally in pancreatic β-cells and liver parenchymal cells. In addition, GK is a rate-controlling enzyme for glucose metabolism in these two cell types that are known to play critical roles in whole-body glucose homeostasis [Chipkin, S.R., Kelly, K.L., and Ruderman, N.B. in *Joslin's Diabetes* (C.R. Khan and G.C. Wier, eds.), Lea and Febiger, Philadelphia, PA, pages 97-115, 1994]. The concentration of glucose at which GK demonstrates half-maximal activity is approximately 8 mM. The other three hexokinases are saturated with glucose at much lower concentrations (<1 mM). Therefore, the flux of glucose through the GK pathway rises as the concentration of glucose in the blood increases from fasting (5 mM) to postprandial (≈10-15 mM) levels following a carbohydrate-containing meal [Printz, R.G., Magnuson, M.A., and Granner, D.K. in *Ann. Rev. Nutrition* Vol. 13 (R.E. Olson, D.M. Bier, and D.B. McCormick, eds.), Annual Review, Inc., Palo Alto, CA, pages 463-496, 1993]. These findings contributed over a decade ago to the hypothesis that GK functions as a glucose sensor in β-cells and hepatocytes (Meglasson, M.D. and Matschinsky, F.M. *Amer. J. Physiol.* 246, E1-E13, 1984). In recent years, studies in transgenic animals have confirmed that GK does indeed play a critical role in whole-body glucose homeostasis. Animals that do not express GK die within days of birth with severe diabetes while animals overexpressing GK have improved glucose tolerance (Grupe, A., Hultgren, B., Ryan, A. et al., *Cell* 83, 69-78, 1995; Ferrie, T., Riu, E., Bosch, F. et al., *FASEB J.*, 10, 1213-1218, 1996). An increase in glucose exposure is coupled through GK in β-cells to increased insulin secretion and in hepatocytes to increased glycogen deposition and perhaps decreased glucose production.

The finding that type II maturity-onset diabetes of the young (MODY-2) is caused by loss of function mutations in the GK gene suggests that GK also functions as a glucose sensor in humans (Liang, Y., Kesavan, P., Wang, L. et al., *Biochem. J.* 309, 167-173, 1995). Additional evidence supporting an important role for GK in the regulation of glucose metabolism in humans was provided by the identification of patients that express a mutant form of GK with increased enzymatic activity. These patients exhibit a fasting hypoglycemia associated with an inappropriately elevated level of plasma insulin (Glaser, B., Kesavan, P., Heyman, M. et al., *New England J. Med.* 338, 226-230, 1998). While mutations of the GK gene are not found in the majority of patients with type II diabetes, compounds that activate GK and, thereby, increase the sensitivity of the GK sensor system will still be useful in the treatment of the hyperglycemia characteristic of all type II diabetes. Glucokinase activators will increase the flux of glucose metabolism in β-cells and hepatocytes, which will be coupled to increased insulin secretion. Such agents would be useful for treating type II diabetes.

In an effort to elucidate the mechanisms underlying kinase activation , the crystal structure of such proteins is often sought to be determined. The crystal structures of several hexokinases have been reported. See, e.g. A. E. Aleshin, C. Zeng, G. P. Bourenkov, H. D. Bartunik, H. J. Fromm & R. B. Honzatko 'The mechanism of regulation of hexokinase: new insights from the crystal structure of recombinant human brain hexokinase complexed with glucose and glucose-6-phosphate' *Structure* 6, 39-50 (1998); W. S. Bennett, Jr. & T. A. Steitz 'Structure of a complex between yeast hexokinase A and glucose I. Structure determination and refinement at 3.5 Å resolution' *J. Mol. Biol.* 140, 183-209 (1978); and S. Ito, S. Fushinobu, I. Yoshioka, S. Koga, H. Matsuzawa & T. Wakagi 'Structural Basis for the ADP-Specificity of a Novel Glucokinase from a Hyperthermophilic Archaeon' *Structure* 9, 205-214 (2001). Despite these reports, researchers armed with the knowledge of how to obtain crystals of related hexokinases have attempted to obtain crystals of any mammalian Glucokinase without success.

Applicants have discovered protocols which allow crystallization of mammalian Glucokinase with or without a bound allosteric ligand. The crystal structure has been solved by X-ray crystallography to a resolution of 2.7 Å. See Figures 3 and 4. Thus the invention relates to a crystalline form of Glucokinase and a crystalline form of a complex of Glucokinase and an allosteric ligand. The invention further relates to a method of forming crystals of Glucokinase, with or without a bound allosteric ligand.

Figure 1 shows Glucokinase co-crystals having P6(5)22 symmetry.

Figure 2 shows the amino acid sequence of an expressed Glucokinase used for crystallization.

Figure 3 shows a ribbon diagram of the structure of Glucokinase showing the α-helices and β-sheets.

Figure 4 shows the atomic structure coordinates for Glucokinase bound to 3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamide.

The present invention relates to crystalline forms of mammalian Glucokinase, with or without a ligand bound in the allosteric site, where the crystals are of sufficient quality and size to allow for the determination of the three-dimensional X-ray diffraction structure to a resolution of about 2.0 Å to about 3.5 Å. The invention also relates to methods for preparing and crystallizing the Glucokinase. The crystalline forms of Glucokinase, as well as information derived from their crystal structures can be used to analyze and modify glucokinase activity as well as to identify compounds that interact with the allosteric site.

The crystals of the invention include apo crystals and co-crystals. The apo crystals of the invention generally comprise substantially pure Glucokinase. The co-crystals generally comprise substantially pure Glucokinase with a ligand bound to the allosteric site.

It is to be understood that the crystalline Glucokinases of the invention are not limited to naturally occurring or native Glucokinases. Indeed, the crystals of the invention include mutants of the native Glucokinases. Mutants of native Glucokinases are obtained by replacing at least one amino acid residue in a native Glucokinase domain with a different amino acid residue, or by adding or deleting amino acid residues within the native polypeptide or at the N- or C- terminus of the native polypeptide, and have substantially the same three-dimensional structure as the native Glucokinase from which the mutant is derived.

By having substantially the same three-dimensional structure is meant having a set of atomic structure coordinates from an apo- or co-crystal that have a root mean square deviation of less than or equal to about 2 Å when superimposed with the atomic structure coordinates of the native Glucokinase from which the mutant is derived when at least about 50% to about 100% of the alpha carbon atoms of the native Glucokinase are included in the superposition.

In some instances, it may be particularly advantageous or convenient to substitute, delete and/or add amino acid residues to a native Glucokinase domain in order to provide convenient cloning sites in cDNA encoding the polypeptide, to aid in purification of the polypeptide, etc. Such substitutions, deletions and/or additions which do not substantially alter the three dimensional structure of the native Glucokinase will be apparent to those having skills in the art.

It should be noted that the mutants contemplated herein need not exhibit glucokinase activity. Indeed, amino acid substitutions, additions or deletions that interfere with the kinase activity of the glucokinase but which do not significantly alter the three-dimensional structure of the domain are specifically contemplated by the invention. Such crystalline polypeptides, or the atomic structure coordinates obtained therefrom, can be used to identify compounds that bind to the native domain. These compounds may affect the activity or the native domain.

The derivative crystals of the invention generally comprise a crystalline glucokinase polypeptide in covalent association with one or more heavy metal atoms. The polypeptide may correspond to a native or a mutated Glucokinase. Heavy metal atoms useful for providing derivative crystals include, by way of example and not limitation, gold and mercury. Alternatively, derivative crystals can be formed from proteins which have heavy atoms incorporated into one or more amino acids, such as seleno-methionine substitutions for methionine.

The co-crystals of the invention generally comprise a crystalline Glucokinase polypeptide in association with one or more compounds at an allosteric site of the polypeptide. The association may be covalent or non-covalent.

The native and mutated glucokinase polypeptides described herein may be isolated from natural sources or produced by methods well known to those skilled in the art of molecular biology. Expression vectors to be used may contain a native or mutated Glucokinase polypeptide coding sequence and appropriate transcriptional and/or translational control signals. These methods include in vitro recombinant DNA techniques, synthetic techniques and in vivo recombination/genetic recombination. See, for example, the techniques described in Maniatis et al., 1989, *Molecular Cloning: A Laboratory Manual*, Cold Spring Harbor Laboratory, NY; and Ausubel et al., 1989, *Current Protocols in Molecular Biology*, Greene Publishing Associates and Wiley Interscience, NY.

A variety of host-expression vector systems may be utilized to express the Glucokinase coding sequence. These include but are not limited to microorganisms such as bacteria transformed with recombinant bacteriophage DNA, plasmid DNA or cosmid DNA expression vectors containing the Glucokinase coding sequence; yeast transformed with recombinant yeast expression vectors containing the Glucokinase coding sequence; insect cell systems infected with recombinant virus expression vectors (e.g. baculovirus) containing the Glucokinase coding sequence; plant cell systems infected with recombinant virus expression vectors (e.g., cauliflower mosaic virus, CaMV; tobacco mosiac virus, TMV) or transformed with recombinant plasmid expression vectors (e.g., Ti plasmid) containing the glucokinase coding sequence; or animal cell systems. The expression elements of these systems vary in their strength and specificities. Depending on the host/vector system utilized, any of a number of suitable transcription and translation elements, including constitutive and inducible promotors such as pL of bacteriophage μ, plac, ptrp, ptac (ptrp-lac hybrid promoter) and the like may be used; when cloning in insect cell systems, promoters such as the baculovirus polyhedrin promoter may be used; when cloning in plant cell systems, promoters derived from the genome of plant cells (e.g., heat shock promoters; the promoter for the small subunit of RUBISCO; the promoter for the chlorophyll a/b binding protein) or from plant viruses (e.g., the 35 S RNA promoter of CaMV; the coat protein promoter of TMV) may be used; when cloning in mammalian cell systems, promoters derived from the genome of mammalian cells (e.g., metallothionein promoter) or from mammalian viruses (e.g., the adenovirus late promoter; the vaccinia virus 7.5K promoter) may be used; when generating cell lines that contain multiple copies of the glucokinase coding sequence, SV40-, BPV- and EBV-based vectors may be used with an appropriate selectable marker.

The apo, derivative and co-crystals of the invention can be obtained by techniques well-known in the art of protein crystallography, including batch, liquid bridge, dialysis, vapor diffusion and hanging drop methods (see e.g. McPherson, 1982, *Preparation and Analysis of Protein Crystals*, John Wiley, NY; McPherson, 1990, *Eur. J. Biochem.* 189:1-23; Webber, 1991, *Adv. Protein Chem.* 41:1-36; Crystallization of Nucleic Acids and Proteins, Edited by Arnaud Ducruix and Richard Giege, Oxford University Press; Protein Crystallization Techniques, Strategies, and Tips, Edited by Terese Bergfors, International University Line, 1999). Generally, the apo- or co-crystals of the invention are grown by

placing a substantially pure Glucokinase polypeptide in an aqueous buffer containing a precipitant at a concentration just below that necessary to precipitate the protein. Water is then removed from the solution by controlled evaporation to produce crystallizing conditions, which are maintained until crystal growth ceases.

In a preferred embodiment of the invention, apo or co-crystals are grown by vapor diffusion. In this method, the polypeptide/precipitant solution is allowed to equilibrate in a closed container with a larger aqueous reservoir having a precipitant concentration optimal for producing crystals. Generally, less than about 10 µL of subtantially pure polypeptide solution is mixed with an equal volume of reservoir solution, giving a precipitant concentration about half that required for crystallization. This solution is suspended as a droplet underneath a coverslip, which is sealed onto the top of a reservoir. The sealed container is allowed to stand, from one day to one year, usually for about 2-6 weeks, until crystals grow.

For crystals of the invention, it has been found that hanging drops containing about 2-5 µl of Glucokinase (9-22 mg/ml in 20 mM tris pH 7.1 measured at room temperature, 50 mM NaCl, 50 mM glucose, 10 mM DTT and optionally 0.2 mM EDTA) and an equal amount of reservoir solution (16-25% w/v polyethylene glycol with an average molecular weight from about 8000 to about 10000 Daltons, 0.1-0.2 M tris or bistris or Hepes or ammonium phosphate buffer, pH 6.9-7.5, 8-10 mM DTT, 0 - 30% saturated glucose) suspended over 0.5 to 1.0 mL reservoir buffer for about 3-4 weeks at 4-6°C provided crystals suitable for high resolution X-ray structure determination. Particularly preferred conditions were: about 2-5 µl of Glucokinase (10 mg/ml in 20 mM tris pH 7.1 measured at room temperature, 50 mM NaCl, 50 mM glucose, 10 mM DTT and optionally 0.2 mM EDTA) and an equal amount of reservoir solution (22.5% w/v polyethylene glycol with an average molecular weight of about 10000 Daltons, 0.1 M tris pH 7.08, 10 mM DTT, 20% glucose) were suspended over 0.5 to 1.0 mL reservoir buffer for about 3-4 weeks at 4-6°C.

The optimum procedure for growing crystals large enough to collect data from involved first streaking 3-4 µl of protein solution on the coverslip, followed by streaking 3-4 µl of well solution across the elongated droplet of protein, forming a droplet shaped like the letter 'X'. Before discovering this crossed droplet technique, most droplets yielded showers of small crystals which were not large enough for data collection purposes. The crossed droplets allow gradients of protein and precipitating agent to form as the two solutions slowly mix, and the resulting kinetics of crystal nucleation and growth are optimal for the growth of a small number of large crystals in each crossed droplet. Simply mixing the protein and precipitant solutions together in a single round droplet often produced an overabundance of nuclei which grew to a final size too small for data collection purposes. Crystals usually appeared within 5 days of setup. The crystals grow in the form of hexagonal bipyramids, reaching dimensions of 0.2 x 0.2 x 0.4 mm typically, although larger crystals are often observed. Figure 1 shows grown crystals.

Crystals may be frozen prior to data collection. The crystals were cryo-protected with either (a) 20-30% saturated glucose present in the crystallization setup, (b) ethanol added to 15-20%, (c) ethylene glycol added to 10-20% and PEG10,000 brought up to 25%, or (d) glycerol added to 15%. The crystals were either briefly immersed in the cryo-protectant or soaked in the cryo-protectant for periods as long as a day. Freezing was accomplished by immersing the crystal in a bath of liquid nitrogen or by placing the crystal in a stream of nitrogen gas at 100 K.

The mosaic spread of the frozen crystals could sometimes be reduced by annealing, wherein the stream of cold nitrogen gas is briefly blocked, allowing the frozen crystal to thaw momentarily before re-freezing in the nitrogen gas stream. Another technique which was sometimes helpful in data collection was to center one of the ends of the hexagonal bipyramid in the x-ray beam, rather than the mid portion of the crystal. The mosaic spread could sometimes be reduced by this technique.

Diffraction data typically extending to 2.7 Å was collected from the frozen crystals at the synchrotron beamline X8C of the National Synchrotron Light Source in Brookhaven, New York. Under optimum conditions, data extending to 2.2 Å was recorded. See Figures 3 and 4 for solution. The space group of the crystals was determined to be P6(5)22 during the course of the solution of the crystal structure. The crystals have unit cell dimensions a = b = 79.62 +/- 0.60 Å, c = 321.73 +/- 3.70 Å, $\alpha\gamma = \beta = 90°$, $\gamma = 120°$. The crystals are in a hexagonal system with P6(5)22 symmetry.

Of course, those having skill in the art will recognize that the above-described crystallization conditions can be varied. Such variations may be used alone or in combination, and include polypeptide solutions containing polypeptide concentrations between 1 mg/mL and 60 mg/mL, any commercially available buffer systems which can maintain pH from about 6.5 to about 7.6, Tris-HCl concentrations between 10 mM and 200 mM, dithiothreitol concentrations between 0 mM and 20 mM, preferably between 8 and 10 mM, substitution of dithiothreitol with beta mercapto ethanol or other art-recognized equivalents, glucose concentrations between 0% w/v and 30% w/v, or substitution of glucose with other sugars known to bind to Glucokinase; and reservoir solutions containing polyethylene glycol (PEG) concentrations between about 10% and about 30%, polyethylene glycol average molecular weights between about 1000 and about 20,000 daltons, any commercially available buffer systems which can maintain pH from about 6.5 to about 7.6, dithiothreitol concentrations between 0 mM and 20 mM, substitution of dithiothreitol with beta mercapto ethanol or other art-recognized -SH group containing equivalents, or substitution of glucose with other sugars known to bind to Glucokinase, and temperature ranges between 4 and 20°C.

Derivative crystals of the invention can be obtained by soaking apo or co-crystals in mother liquor containing salts of heavy metal atoms, according to procedures known to those of skill in the art of X-ray crystallography.

Co-crystals of the invention can be obtained by soaking an apo crystal in mother liquor containing a ligand that binds to the allosteric site, or can be obtained by co-crystallizing the Glucokinase polypeptide in the presence of one or more ligands that bind to the allosteric site. Preferably, co-crystals are formed with a glucokinase activator disclosed in US Pat. No. 6,320,050; US Pat. Appl. 09/532,506 filed March 21, 2000; US Pat. Appl. 09/675,781 filed September 28, 2000; US Pat. Appl. 09/727,624, filed December 1, 2000; US Pat. Appl. 09/841,983, filed April 25, 2001; US Pat. Appl. 09/843,466, filed April 26, 2001; US Pat. Appl. 09/846,820, filed May 1, 2001; US Pat. Appl. 09/846,821, filed May 1, 2001; US Pat. Appl. 09/905,152, filed July 13, 2001; US Pat. Appl. 09/924,247, filed August 8, 2001; US Provisional Pat. Appl. 60/251,637, filed December 6, 2000; or US Provisional Pat. Appl. 60/318,715, filed September 13, 2001, each of which is incorporated herein by reference.

Methods for obtaining the three-dimensional structure of the crystalline glucokinases described herein, as well as the atomic structure coordinates, are well-known in the art (see, e.g., D. E. McRee, Practical Protein Crystallography, published by Academic Press, San Diego (1993), and references cited therein).

The crystals of the invention, and particularly the atomic structure coordinates obtained therefrom, have a wide variety of uses. For example, the crystals and structure coordinates described herein are particularly useful for identifying compounds that activate Glucokinases as an approach towards developing new therapeutic agents. One such compound is 3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamide and pharmaceutically acceptable salts thereof. Pharmaceutical compositions of said compounds can be developed, and said compounds can be used for the manufacture of a medicament comprising said compound for the treatment of hyperglycemia in type II diabetes.

The structure coordinates described herein can be used as phasing models in determining the crystal structures of additional native or mutated glucokinases, as well as

the structures of co-crystals of such glucokinases with allosteric inhibitors or activators bound. The structure coordinates, as well as models of the three-dimensional structures obtained therefrom, can also be used to aid the elucidation of solution-based structures of native or mutated glucokinases, such as those obtained via NMR. Thus, the crystals and atomic structure coordinates of the invention provide a convenient means for elucidating the structures and functions of glucokinases.

For purposes of clarity and discussion, the crystals of the invention will be described by reference to specific Glucokinase exemplary apo crystals and co-crystals. Those skilled in the art will appreciate that the principles described herein are generally applicable to crystals of any mammalian Glucokinase, including, but not limited to the Glucokinase of Figure 2.

As used herein, "allosteric site" refers in general to any ligand binding site on a mammalian Glucokinase other than the active site of the enzyme.

As used herein, "apo crystal" refers to crystals of mammalian Glucokinase formed without a bound allosteric ligand.

As used herein, "allosteric ligand" refers to any molecule which specifically binds an allosteric site on a mammalian Glucokinase.

EXAMPLES

Example 1: Expression and Purification of Glucokinase

Expression of GK

Glucokinase (GK) was expressed as a glutathione S-transferase (GST) fusion protein in *Escherichia coli*. The amino-acid sequence of the fusion protein is given in Figure 2. The expression construct is based on the pGEX-3X vector from Pharmacia, as described in Y. Liang, P. Kesavan, L. Wang, K. Niswender, Y. Tanizawa, M. A. Permutt, M. A. Magnuson, F. M. Matschinsky, *Biochem. J.* 309, 167 (1995). The construct codes for one of the two liver isozymes of human GK. The GST tag is at the N-terminus of the construct, and is separated from the coding sequence for GK by a Factor Xa cleavage site. After purification of the GST fusion protein, the GST fusion tag was removed with Factor Xa protease, which also removes five residues from the N-terminus of GK.

Purification of GK

E. coli cells expressing GST-GK were suspended in lysis buffer (50 mM tris, 200 mM NaCl, 5 mM EDTA, 5 mM DTT, 1% NP-40, pH 7.7) in the presence of protease inhibitors, incubated with lysozyme at 200 μ/ml for 30 minutes at room temperature, and sonicated 4x30 sec. at 4° C. After centrifugation to remove insoluble material, the supernatant was loaded onto glutathione-Sepharose, washed with lysis buffer and then with lysis buffer minus NP-40. GST-GK was eluted with lysis buffer (minus NP-40) containing 50 mM D-glucose and 20 mM glutathione. The eluted protein was concentrated and dialyzed into 20 mM tris, 100 mM NaCl, 0.2 mM EDTA, 50 mM D-glucose, 1mM DTT, pH 7.7. Factor Xa was added at a protein ratio of 1:100 GST-GK followed by the addition of $CaCl_2$ to 1 mM, and the sample was incubated at 4° C for 48

hours. The sample was added to glutathione Sepharose and the unbound fraction collected and concentrated. The sample was then incubated with benzamidine Sepharose to remove Factor Xa, and the unbound fraction was collected and loaded on a Q Sepharose column equilibrated with 25 mM bis-tris propane, 50 mM NaCl, 5 mM DTT, 50 mM D-glucose and 5% glycerol (pH 7.0). The protein was eluted with a NaCl gradient from 50-400 mM. Fractions containing purified GK were pooled and concentrated and filtered.

Example 2: Formation of apo Crystal

4 µl of glucokinase and 4 µl of precipitant were mixed and equilibrated against the precipitant solution at 4° C. The glucokinase solution consisted of 22 mg/ml glucokinase prepared in Example 1 in 20 mM hepes pH 7.5, 50 mM NaCl, 10 mM DTT, and 50 mM glucose. The precipitant consisted of 22.5% PEG10000, 0.1 M tris pH 7.08, 10 mM DTT, 20% glucose; the precipitant solution contained seed crystals in order to microseed the droplets. Crystals appeared in the droplets after leaving the crystallization plates at 4° C.

Example 3: Formation of Co-crystal with 3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamide

3(a):

4 µl of glucokinase and 4 µl of precipitant were mixed and equilibrated against the precipitant solution at 4° C. The glucokinase solution consisted of 13 mg/ml glucokinase prepared in Example 1 in 20 mM tris pH 7.0, 50 mM NaCl, 10 mM DTT, 50 mM glucose, and the glucokinase activator 3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamide at a concentration 5 times that of the protein. The precipitant consisted of 22.5% PEG10000, 0.1 M tris pH 7.08, 10 mM DTT, 20% glucose. Crystals appeared in the droplets after leaving the crystallization plates at 4° C.

3(b):

Alternatively, crystals were grown as in Example 3(a) with the following changes: instead of 4 µl glucokinase and 4 µl precipitant, 2 µl of each were used; the glucokinase solution contained 11 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 22.5% PEG10000 as precipitant 18% PEG8000 was used; the precipitant solution contained seed crystals in order to microseed the droplets.

3(c):

In another alternative, crystals were grown as in Example 3(a) with the following changes: instead of 4 µl glucokinase and 4 µl precipitant, 2 µl of each were used; the glucokinase solution contained 11 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 22.5% PEG10000 as precipitant 20% PEG8000 was used; the precipitant solution contained seed crystals in order to microseed the droplets.

3(d):

In yet another alternative, crystals were grown as in Example 3(a) with the following changes: instead of 4 µl glucokinase and 4 µl precipitant, 2 µl of each were used; the glucokinase solution contained 12 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 22.5% PEG10000 as precipitant 16% PEG10000 was used; glucose was not present as a component of the precipitant; the precipitant solution contained seed crystals in order to microseed the droplets.

3(e):

In still another alternative, crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 11 mg/ml glucokinase in tris

buffer at pH 7.1 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 22.5% PEG10000 as precipitant 25% PEG10000 was used.

3(f):

In still another alternative, crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 11 mg/ml glucokinase in tris buffer at pH 7.1 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 22.5% PEG10000 as precipitant 21.25% PEG10000 was used; in place of tris buffered at pH 7.08 in the precipitant tris buffered at pH 7.52 was used.

3(g):

In still another alternative, crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 12 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of tris buffered at pH 7.08 in the precipitant, hepes buffered at pH 6.89 was used; in place of 20% glucose in the precipitant, 200 mM glucose was used.

3(h):

In still another alternative, crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 12 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 0.1 M tris buffered at pH 7.08 in the precipitant, 0.2 M ammonium phosphate buffered at pH 7.03 was used; in place of 20% glucose in the precipitant, 200 mM glucose was used.

3(i):

In still another alternative, crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 10 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 22.5% PEG10000 as precipitant, 20% PEG10000 was used; in place of tris buffered at pH 7.08 in the precipitant, tris buffered at pH 7.05 was used; in place of 10 mM DTT in the precipitant, 8 mM DTT was used; glucose was not present as a component of the precipitant.

3(j):

In still another alternative, crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 12 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 22.5% PEG10000 as precipitant, 22% PEG8000 was used; glucose was not present as a component of the precipitant; the precipitant solution contained seed crystals in order to microseed the droplets.

3(k):

In still another alternative, crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 11 mg/ml glucokinase in tris buffer at pH 7.1 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of 20% glucose in the precipitant, 30% glucose was used.

Example 4: Formation of Co-crystal with N-(5-Bromo-pyridin-2-yl)-2-(3-chloro-4-methanesulfonyl-phenyl)-3-cyclopentyl-propionamide

Crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 9 mg/ml glucokinase in tris buffer at pH 7.1 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of the glucokinase activator of Example 3(a), the glucokinase solution contained the glucokinase activator N-(5-Bromo-pyridin-2-yl)-2-(3-chloro-4-methanesulfonyl-phenyl)-3-cyclopentyl-propionamide; in place of 20% glucose in the precipitant, 200 mM glucose was used.

Example 5: Formation of Co-crystal with 2-(3-Chloro-4-methanesulfonyl-phenyl)-3-cyclopentyl-N-(5-trifluoromethyl-pyridin-2-yl)-propionamide

Crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 10 mg/ml glucokinase in tris buffer at pH 7.1 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of the glucokinase

activator of Example 3(a), the glucokinase solution contained the glucokinase activator 2-(3-Chloro-4-methanesulfonyl-phenyl)-3-cyclopentyl-N-(5-trifluoromethyl-pyridin-2-yl)-propionamide; in place of 22.5% PEG10000 as precipitant, 21.25% PEG10000 was used.

Example 6: Formation of Co-crystal with (2S)-2-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionylamino]-thiazole-4-carboxylic acid methyl ester

Crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 10 mg/ml glucokinase in tris buffer at pH 7.1 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of the glucokinase activator of Example 3(a), the glucokinase solution contained the glucokinase activator (2S)-2-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionylamino]-thiazole-4-carboxylic acid methyl ester; in place of 22.5% PEG10000 as precipitant, 21.25% PEG10000 was used; in place of tris buffered at pH 7.08 in the precipitant, bistris buffered at pH 7.0 was used.

Example 7: Formation of Co-crystal with (2S)-{2-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionylamino]-thiazol-5-yl}-oxo-acetic acid ethyl ester

Crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 10 mg/ml glucokinase in tris buffer at pH 7.1 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of the glucokinase activator of Example 3(a), the glucokinase solution contained the glucokinase activator (2S)-{2-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionylamino]-thiazol-5-yl}-oxo-acetic acid ethyl ester; in place of 22.5% PEG10000 as precipitant, 21.25% PEG10000 was used.

Example 8: Formation of Co-crystal with (2S)-{3-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionyl]-ureido}-acetic acid methylester

Crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 9 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of the glucokinase activator of Example 3(a), the glucokinase solution contained the glucokinase activator (2S)-{3-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionyl]-ureido}-acetic acid methylester; in place of 20% glucose in the precipitant, 200 mM glucose was used.

Example 9: Formation of Co-crystal with (2S)-1-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionyl]-3-(3-hydroxy-propyl)-urea

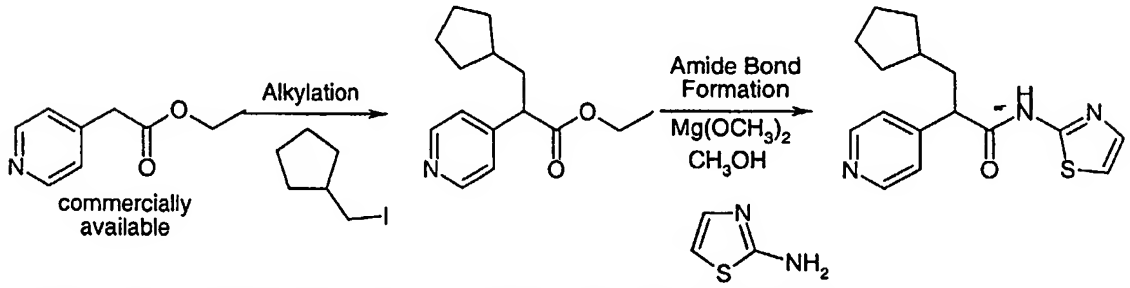
Crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 14 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of the glucokinase activator of Example 3(a), the glucokinase solution contained the glucokinase activator (2S)-1-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionyl]-3-(3-hydroxy-propyl)-urea; in place of 20% glucose in the precipitant, 200 mM glucose was used.

Example 10: Formation of Co-crystal with (2S)-{3-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionyl]-ureido}-acetic acid ethyl ester

Crystals were grown as in Example 3(a) with the following changes: the glucokinase solution contained 14 mg/ml glucokinase in tris buffer at pH 7.08 instead of 7.0; the glucokinase solution included 0.2 mM EDTA; in place of the glucokinase activator of Example 3(a), the glucokinase solution contained the glucokinase activator (2S)-{3-[3-Cyclopentyl-2-(3,4-dichloro-phenyl)-propionyl]-ureido}-acetic acid ethyl ester; in place of tris buffered at pH 7.08 in the precipitant, tris buffered at pH 7.05 was used.

Example 11: Synthesis of 3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamide

3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamide can be prepared using well-



known organic synthesis techniques according to the following reaction scheme:

3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamide is useful as an allosteric activator of Glucokinase and to assist the formation of co-crystals of Glucokinase.

In the present specification "comprises" means "includes or consists of" and "comprising" means "including or consisting of".

The features disclosed in the foregoing description, or the following claims, or the accompanying drawings, expressed in their specific forms or in terms of a means for performing the disclosed function, or a method or process for attaining the disclosed result, as appropriate, may, separately, or in any combination of such features, be utilised for realising the invention in diverse forms thereof.

SEQUENCE LISTING

<110> F. Hoffmann - La Roche

<120> CRYSTALS OF GLUCOKINASE AND METHODS OF GROWING THEM

<130> Case 20892

<140> US 60/341988

<141> 2001-12-19

<150> US 60/341988

<151> 2001-12-19

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<170> PatentIn version 3.1

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690

Claims

1. A co-crystal of mammalian Glucokinase and a ligand bound to an allosteric site of the Glucokinase, wherein

the co-crystal has unit cell dimensions of:

a and b are from 79.02 Å to 80.22 Å;

c is from 318.03 Å to 325.03 Å;

α and β are 90°; and

γ is 120°;

and the co-crystal has P6(5)22 symmetry.

2. A crystal of mammalian Glucokinase, wherein

the crystal has unit cell dimensions of:

a and b are from 79.02 Å to 80.22 Å;

c is from 318.03 Å to 325.03 Å;

α and β are 90°; and

γ is 120°;

and the crystal has P6(5)22 symmetry.

3. A process for co-crystalizing mammalian Glucokinase and an allosteric ligand of Glucokinase, the process comprising:

providing a buffered, aqueous solution of 9 to 22 mg/ml of the mammalian Glucokinase;

adding a molar excess of the allosteric ligand to the aqueous solution of mammalian Glucokinase; and

growing crystals by vapor diffusion using a buffered reservoir solution between about 10% and about 30% PEG, about 0% w/v and about 30% w/v glucose, and between 0 and 20 mM DTT, wherein the PEG has an average molecular weight between about 1,000 and about 20,000.

4. The process of claim 3, wherein the step of growing crystals by vapor diffusion comprises:

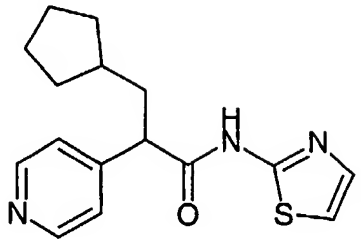
streaking the buffered, aqueous solution of mammalian Glucokinase with added allosteric ligand on a surface to form an elongated droplet of protein solution, and

streaking about an equal amount of the buffered reservoir solution across the elongated droplet of protein solution, forming a combined droplet shaped like the letter 'X'.

5. A crystal produced by the process of claims 3 or 4.

6. A compound identified by analysing the structure coordinates of the co-crystal of claim 1, said compound being a ligand that binds to the allosteric site of Glucokinase.

7. The compound



and pharmaceutically acceptable salts thereof.

8. A pharmaceutical composition comprising the compound of claim 6.

9. The pharmaceutical composition of claim 8, wherein said compound is the compound of claim 7.

10. Use of the compound of claim 6 for the manufacture of a medicament comprising a compound according to claim 6 for the treatment of hyperglycemia in type II diabetes.

11. The use of claim 10 wherein said compound is the compound of claim 7.

12. A compound according to claims 6 or 7, for use as a therapeutic active substance, in particular for the reduction of hyperglycemia in type II diabetes.

13. The novel crystals, processes, compounds, compositions and uses as hereinbefore described.

14. A process according to Claim 3 or 4 further comprising the step of freezing the crystals.

15. A method of identifying a ligand that binds to the allosteric site of Glucokinase comprising analysing the structure co-ordinates of a co-crystal according to Claim 1.

16. Use of a co-crystal according to Claim 1 or a crystal according to Claim 2 in the identification of a compound which activates Glucokinase.

17. Use of a co-crystal according to Claim 1 or a crystal according to Claim 2 for elucidating the structure and function of a Glucokinase.

18. A compound according to Claim 6 or 7, or a composition according to Claim 8 or 9, for use in a method of treatment of human or animal body.

19. Any novel feature or combination of features described herein.

Application No:	GB 0229456.9	**Examiner:**	Dr Rowena Dinham
Claims searched:	1-5 & 14-17; and 12, 13, 18 and 19 (in part)	**Date of search:**	16 June 2003

Patents Act 1977 : Search Report under Section 17

Documents considered to be relevant:

Category	Relevant to claims	Identity of document and passage or figure of particular relevance
A, P		*Protein Science*; Vol 11, pp 2456-2463 (2002). Tsuge *et al.* "*Crystal structure of the ADP-dependent glucokinase...*" See entire document, especially Results and Discussion "*Overall strucure*"
A		*Structure*; Vol 9, pp 205-214 (2001). Ito *et al.* "*Structural basis for the ADP-specificity of a novel glucokinase...*" See entire document, especially Results and Discussion "*Crystal structure of* T. lioralis *glucokinase*"
A		*Diabetes*; Vol 48, pp 1698-1705 (1999). Mahalingam *et al.* "*Structural model of human glucokinase...*" See entire document, especially Results "*Overall model and comparison with previous model and hexokinase structures*"

Categories:

X	Document indicating lack of novelty or inventive step	A	Document indicating technological background and/or state of the art.
Y	Document indicating lack of inventive step if combined with one or more other documents of same category.	P	Document published on or after the declared priority date but before the filing date of this invention.
&	Member of the same patent family	E	Patent document published on or after, but with priority date earlier than, the filing date of this application.

Field of Search:

Search of GB, EP, WO & US patent documents classified in the following areas of the UKC[V]:

Worldwide search of patent documents classified in the following areas of the IPC[7]:

C12N; C30B; G06F

The following online and other databases have been used in the preparation of this search report:

WPI, EPODOC, JAPIO, MEDLINE, BIOSIS, EMBASE, SCISEARCH, CAPLUS